Felix Finster
Johannes Kleiner
Christian Röken
Jürgen Tolksdorf
Editors

Quantum Mathematical Physics

A Bridge between Mathematics and Physics

Birkhäuser

Quantum Mathematical Physics

Felix Finster • Johannes Kleiner • Christian Röken •
Jürgen Tolksdorf
Editors

Quantum Mathematical Physics

A Bridge between Mathematics and Physics

Birkhäuser

Editors
Felix Finster
Fakultät für Mathematik
Universität Regensburg
Regensburg, Germany

Johannes Kleiner
Fakultät für Mathematik
Universität Regensburg
Regensburg, Germany

Christian Röken
Fakultät für Mathematik
Universität Regensburg
Regensburg, Germany

Jürgen Tolksdorf
MPI für Mathematik in den Naturwissenschaften
Leipzig, Germany

ISBN 978-3-319-26900-9 ISBN 978-3-319-26902-3 (eBook)
DOI 10.1007/978-3-319-26902-3

Library of Congress Control Number: 2015957955

Mathematics Subject Classification (2010): 81-06, 83-06, 81T20, 81T70, 81T75, 81T15, 35Q40, 83C45, 35L10

Springer Cham Heidelberg New York Dordrecht London

Preface

The present volume is based on the international conference *Quantum Mathematical Physics – A Bridge between Mathematics and Physics* that was held at the University of Regensburg (Germany) from September 29 to October 2, 2014. This conference was a successor of similar international conferences which took place at the *Heinrich-Fabri Institute* (Blaubeuren) in 2003 and 2005, at the *Max Planck Institute for Mathematics in the Sciences* (Leipzig) in 2007 and at the *University of Regensburg* in 2010. The basic intention of this series of conferences is to bring together mathematicians and physicists to discuss profound questions in quantum field theory and gravity. More specifically, the series aims at discussing concepts which underpin different mathematical and physical approaches to quantum field theory and gravity.

Since the invention of general relativity and quantum mechanics at the beginning of the twentieth century, physicists made an enormous effort to incorporate gravity and quantum physics into a unified framework. In doing so, many approaches have been developed to overcome the basic conceptual and mathematical differences between quantum theory and general relativity. Moreover, both quantum theory and general relativity have their own problems and shortcomings. It turns out that many of these problems are related to each other and to the problem of the unification of quantum theory and gravity. The aim of the conference was to shed light on these problems and to indicate possible solutions.

On one hand, general relativity describes systems on large scales (like the solar system, galaxies, and cosmological phenomena). This is reflected in the fact that in general relativity, space-time has locally the simple structure of Minkowski space, whereas gravitational effects usually show up in the large-scale geometry. Under generic assumptions, there are phenomena like black holes and cosmological singularities which are not yet understood in a physically satisfying way. Quantum theory, on the other hand, usually describes systems on small scales (like atoms, nuclei, or elementary particles). Indeed, on small scales the Heisenberg uncertainty principle becomes relevant and quantum effects come into play. One of the open problems is that there is no satisfying mathematical description of interacting quantum fields.

One of the fundamental difficulties in combining gravity with quantum physics lies in the fact that general relativity is a theory on the dynamics of space-time itself, whereas quantum theory usually aims to describe the dynamics of matter within a given space-time background (in the simplest case by Minkowski space). Moreover, the geometric description of general relativity makes it necessary to describe objects locally in an arbitrary small neighborhood of a point. But localizing quantum mechanical wave functions to such a small neighborhood, the Heisenberg uncertainty principle gives rise to large energy fluctuations. Considering these energy fluctuations as a gravitational source, one obtains a contradiction to the above picture that gravity comes into play only on large scales. Thus, although both theories are experimentally well confirmed, they seem to conceptually contradict each other. This incompatibility also becomes apparent in the mathematical formulation: From a mathematical perspective, general relativity is usually regarded as a purely geometric theory. However, quantum physics is described mathematically in an algebraic and functional analytic language.

There are various approaches to overcome these issues. For instance, in string theory one replaces point-like particles by one-dimensional objects. Other approaches, like loop quantum gravity, causal fermion systems, or noncommutative geometry, rely on the assumption that the macroscopic smooth space-time structure should emerge from more fundamental structures on the microscopic scale. Alternatively, one tries to treat interacting theories as "effective theories" or considers quantum theory from an axiomatic and categorical view point in a way that allows to incorporate the concept of local observers. Most of these modern mathematical approaches to unify quantum physics with general relativity have the advantage to combine geometric structures with algebraic and functional analytic methods. Some of these "quantum mathematical concepts" are discussed in the present conference volume.

The carefully selected and refereed articles in this volume either give a survey or focus on specific issues. They explain the state of the art of various rigorous approaches to quantum field theory and gravity. Most of the articles are based on talks at the abovementioned conference. All talks of the conference were recorded, and most are available online at

http://www.ur.de/qft2014.

For the first time, the conference included two evening talks devoted to new experimental developments (dark matter/energy and the Higgs particle). It was again a main purpose of the conference to set the stage for stimulating discussions. To this end, extra time slots were reserved for panel and plenary discussions. Here is a list of some of the questions raised in the discussions:

1. **Quantum gravity:** What should a physically convincing theory of quantum gravity accomplish? Which are the most promising directions to find such a theory of quantum gravity? Why does one need to "quantize" gravity – is it not sufficient to describe it classically? How important is mathematical consistency?
2. **Quantization:** Do quantum field theories necessarily arise by quantizing a classical field theory? Is such a quantization procedure necessary in order to

have a physical interpretation of the resulting quantum field theory? Does it make physical sense to quantize pure gravity without matter?
3. **Future perspectives:** Which directions in mathematical physics seem most promising for young researchers to work on? Is it recommendable for young researchers to study new topics or should they rather work on well-established problems? Which are the big challenges for mathematical physics in the next years?
4. **Axiomatic frameworks:** Do the various axiomatic frameworks (such as algebraic quantum field theory, causal fermion systems, noncommutative geometry, etc.) offer a suitable framework for unifying gravity and quantum theory? Can causality be expected to hold?
5. **Dark energy and dark matter:** Is dark energy related to quantum field theoretic effects like vacuum fluctuations? Or do the explanations of dark energy and dark matter require new physical concepts? Should dark matter and dark energy be considered as some kind of "matter" or "field" in space-time?
6. **Mathematics of future theories:** Which contemporary mathematical developments might play an important role in the formulation of new physical theories?

We are grateful to Klaus Fredenhagen (Hamburg), José Maria Gracia-Bondia (Madrid), Gerhard Börner (München), and Harald Grosse (Wien) for contributing to the discussions as members of the panel. The discussions were moderated by Johannes Kleiner.

Regensburg, Germany — Felix Finster
Johannes Kleiner
Christian Röken
Leipzig, Germany — Jürgen Tolksdorf
July 2015

Acknowledgments

It is a great pleasure for us to thank all participants for their contributions which made the conference so successful. We are very grateful to the staff of the Department of Mathematics of the University of Regensburg, especially to Eva Rütz, who managed the administrative work before, during, and after the conference excellently. Also, we would like to thank Dieter Piesch and the group of the Mediathek Regensburg for the excellent video recordings of the talks held at the conference.

We would like to express our deep gratitude to the German Science Foundation (DFG); the Leopoldina National Academy of Sciences; the Max Planck Institute for Mathematics in the Sciences, Leipzig; the International Association of Mathematical Physics (IAMP), the "Regensburger Universitätsstiftung Hans Vielberth"; and the Institute of Mathematics at the University of Regensburg for their generous financial support.

We would like to thank Eberhard Zeidler for his continuous encouragement and support. With his personal engagement and his scientific input, he helped us very much to make this conference possible.

Contents

On the Spin-Statistics Connection in Curved Spacetimes

Christopher J. Fewster

Contents

Abstract The connection between spin and statistics is examined in the context of locally covariant quantum field theory. A generalization is proposed in which locally covariant theories are defined as functors from a category of framed spacetimes to a category of $*$-algebras. This allows for a more operational description of theories with spin, and for the derivation of a more general version of the spin-statistics connection in curved spacetimes than previously available. The proof involves a "rigidity argument" that is also applied in the standard setting of locally covariant quantum field theory to show how properties such as Einstein causality can be transferred from Minkowski spacetime to general curved spacetimes.

Keywords Quantum field theory in curved spacetimes • Spin-statistics connection • Local covariance.

Mathematics Subject Classification (2010). 81T05, 81T20, 81P99.

C.J. Fewster (✉)
Department of Mathematics, University of York, Heslington, York YO10 5DD, UK
e-mail: chris.fewster@york.ac.uk

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_1

1 Introduction

> In conclusion we wish to state, that according to our opinion the connection between spin and statistics is one of the most important applications of the special relativity theory.
> W. Pauli, in [33].

It is an empirical fact that observed elementary particles are either bosons of integer spin, or fermions of half-integer spin. Explanations of this connection between spin and statistics have been sought since the early days of quantum field theory. Fierz [19] and Pauli [33] investigated the issue in free field theories, setting in train a number of progressively more general results. The rigorous proof of a connection between spin and statistics was an early and major achievement of the axiomatic Wightman framework; see [5, 30] and the classic presentation in [38]. Similarly, general results have been proved in the Haag–Kastler framework [23], for example, [8, 9, 22]. In these more algebraic settings, statistics is not tied to the properties of particular fields, but is understood in terms of the graded commutativity of local algebras corresponding to spacelike-separated regions [9], or the properties of super-selection sectors [8, 22].

Nonetheless, the theoretical account of the spin-statistics connection is subtle and even fragile. Nonrelativistic models of quantum field theory are not bound by it, and as Pauli observed [33], one may impose bosonic statistics on a Dirac field at the cost of sacrificing positivity of the Hamiltonian. Ghost fields introduced in gauge theories violate the connection, but also involve indefinite inner products. The rigorous proofs therefore rely on Hilbert space positivity and energy positivity. Moreover, they make essential use of the Poincaré symmetry group and its complex extension together with analyticity properties of the vacuum n-point functions. The spin-statistics connection observed in nature, however, occurs in a spacetime which is not Minkowski space and indeed has no geometrical symmetries. There is neither a global notion of energy positivity (or, more properly, the spectrum condition) nor do we expect n-point functions in typical states of interest on generic spacetimes to have analytic extensions. Thus the general proofs mentioned have no traction and it is far from clear how they can be generalized: a priori it is quite conceivable that the theoretical spin-statistics connection is an accident of special relativity that is broken in passing to the curved spacetimes of general relativity. Indeed, for many years, work on the spin-statistics connection in curved spacetimes was restricted to demonstrations that free models become inconsistent on general spacetimes if equipped with the wrong statistics (e.g., imposing anticommutation relations on a scalar field) [32, 41] unless some other important property such as positivity is sacrificed [24].

The breakthrough was made by Verch [39], who established a general spin-statistics theorem for theories defined on each spacetime by a single field which, in particular, obeys Wightman axioms in Minkowski space. Together with [27], this paper was responsible for laying down many of the foundations of what has

become the locally covariant framework for QFT in curved spacetimes [2]. Verch's assumptions allow certain properties of the theory on one spacetime to be deduced from its properties on another, provided the spacetimes are suitably related by restrictions or deformations of the metric. In particular, the spin-statistics connection is proved by noting that if it were violated in any one spacetime, it would be violated in Minkowski space, contradicting the classic spin-statistics theorem.

Nonetheless, there are good reasons to revisit the spin-statistics connection in curved spacetime. First, as a matter of principle, one would like to gain a better understanding of why spin is the correct concept to investigate in curved spacetime, given the lack of the rotational symmetries that are so closely bound up with the description of spin in Minkowski space. A second, related, point is that [39] describes spinor fields as sections of various bundles associated to the spin bundle. While this is conventional wisdom in QFT in CST, it has the effect of basing the discussion on geometric structures that are, in part, unobservable. This is not a great hindrance if the aim is to discuss a particular model such as the Dirac field. However, we wish to understand the spin-statistics connection for general theories, without necessarily basing the description on fields at all. With that goal in mind, one needs a more fundamental starting point that avoids the insertion of spin by hand. Third, the result proved in [39] is confined to theories in which the algebra in each spacetime is generated by a single field, and the argument is indirect in parts. The purpose of this contribution is to sketch a new and operationally well-motivated perspective on the spin-statistics connection in which spin emerges as a natural concept in curved spacetimes, and which leads to a more general and direct proof of the connection. In particular, there is no longer any need to describe the theory in terms of one or more fields. Full details will appear shortly [10].

The key ideas are (a) a formalisation of the reasoning underlying [39] as a 'rigidity argument', and (b) a generalization of locally covariant QFT based on a category of spacetimes with global coframes (i.e., a 'rods and clocks' account of spacetime measurements). As in [39] the goal is to prove that a spin-statistics connection in curved spacetime is implied by the standard results holding in Minkowski space; however, the proof becomes quite streamlined in the new formulation. We begin by describing the standard version of locally covariant QFT, describing the rigidity argument and some of its other applications in that context, before moving to the discussion of framed spacetimes and the spin-statistics theorem.

2 Locally Covariant QFT

Locally covariant QFT is a general framework for QFT in curved spacetimes, due to Brunetti, Fredenhagen and Verch (BFV) [2], which comprises three main assumptions. The first is the assertion that any quantum field theory respecting locality and covariance can be described by a covariant functor $\mathscr{A} : \mathsf{Loc} \to \mathsf{Alg}$

from the category of globally hyperbolic spacetimes Loc to a category Alg of unital $*$-algebras.[1]

This assumption already contains a lot of information and we shall unpack it in stages, beginning with the spacetimes. Objects of Loc are oriented and time-oriented globally hyperbolic spacetimes (of fixed dimension n) and with finitely many components.[2] Morphisms between spacetimes in Loc are *hyperbolic embeddings*, i.e., isometric embeddings preserving time and space orientations with causally convex image.

The category Alg has objects that are unital $*$-algebras, with morphisms that are injective, unit-preserving $*$-homomorphisms. The functoriality condition requires that the theory assigns an object $\mathscr{A}(\boldsymbol{M})$ of Alg to each spacetime $\boldsymbol{M}$ of Loc, and, furthermore, that each hyperbolic embedding of spacetimes $\psi : \boldsymbol{M} \to \boldsymbol{N}$ is mirrored by an embedding of the corresponding algebras $\mathscr{A}(\psi) : \mathscr{A}(\boldsymbol{M}) \to \mathscr{A}(\boldsymbol{N})$, such that

$$\mathscr{A}(\mathrm{id}_{\boldsymbol{M}}) = \mathrm{id}_{\mathscr{A}(\boldsymbol{M})} \quad \text{and} \quad \mathscr{A}(\varphi \circ \psi) = \mathscr{A}(\varphi) \circ \mathscr{A}(\psi) \tag{1}$$

for all composable embeddings φ and ψ.

Despite its somewhat formal expression, this assumption is well-motivated from an operational viewpoint[3] and provides a natural generalization of the Haag–Kastler–Araki axiomatic description of quantum field theory in Minkowski space. Indeed, as emphasized by BFV, this single assumption already contains several distinct assumptions of the Minkowski framework.

The next ingredient in the BFV framework is the *kinematic net* indexed by $\mathcal{O}(\boldsymbol{M})$, the set of all open causally convex subsets of $\boldsymbol{M}$ with finitely many connected components. Each nonempty $O \in \mathcal{O}(\boldsymbol{M})$ can be regarded as a spacetime $\boldsymbol{M}|_O$ in its own right, by restricting the causal and metric structures of $\boldsymbol{M}$ to O, whereupon the inclusion map of O into the underlying manifold $\boldsymbol{M}$ induces a Loc morphism $\iota_O : \boldsymbol{M}|_O \to \boldsymbol{M}$ (see Fig. 1). The theory $\mathscr{A}$ therefore assigns an algebra $\mathscr{A}(\boldsymbol{M}|_O)$ and an embedding of this algebra into $\mathscr{A}(\boldsymbol{M})$, and we define the kinematic subalgebra to be the image

$$\mathscr{A}^{\mathrm{kin}}(\boldsymbol{M}; O) := \mathscr{A}(\iota_O)(\mathscr{A}(\boldsymbol{M}|_O)). \tag{2}$$

As mentioned above, the net $O \mapsto \mathscr{A}^{\mathrm{kin}}(\boldsymbol{M}; O)$ is the appropriate generalization of the net of local observables studied in Minkowski space AQFT. Some properties are

[1] Other target categories are often used, e.g., the unital C^*-algebra category C*-Alg, and other types of physical theory can be accommodated by making yet other choices.

[2] It is convenient to describe the orientation by means of a connected component of the set of nonvanishing n-forms, and likewise to describe the time-orientation by means of a connected component of the set of nonvanishing timelike 1-form fields. Our signature convention throughout is $+ - \cdots -$.

[3] For a discussion of how the framework can be motivated on operational grounds (and as an expression of 'ignorance principles') see [13, 15].

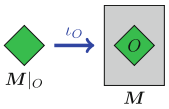


Fig. 1 Schematic illustration of the kinematic net

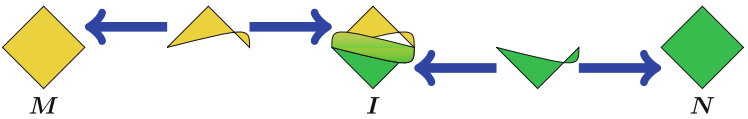


Fig. 2 Schematic representation of spacetime deformation

automatic. For instance, the kinematic algebras are covariantly defined, in the sense that

$$\mathscr{A}^{\mathrm{kin}}(\boldsymbol{N}; \psi(O)) = \mathscr{A}(\psi)(\mathscr{A}^{\mathrm{kin}}(\boldsymbol{M}; O)) \tag{3}$$

for all morphisms $\psi : \boldsymbol{M} \to \boldsymbol{N}$ and all nonempty $O \in \mathcal{O}(\boldsymbol{M})$. This is an immediate consequence of the definitions above and functoriality of $\mathscr{A}$. Similarly spacetime symmetries of $\boldsymbol{M}$ are realised as automorphisms of the kinematic net in a natural way.

It is usual to assume two additional properties. First, the theory obeys *Einstein causality* if, for all causally disjoint $O_1, O_2 \in \mathcal{O}(\boldsymbol{M})$ (i.e., no causal curve joins O_1 to O_2), the corresponding kinematic algebras commute elementwise. Second, $\mathscr{A}$ is said to have the *timeslice property* if it maps every *Cauchy morphism*, i.e., a morphism whose image contains a Cauchy surface of the ambient spacetime, to an isomorphism in Alg. This assumption encodes the dynamics of the theory and plays an important role in allowing the instantiations of $\mathscr{A}$ on different spacetimes to be related. In fact, two spacetimes $\boldsymbol{M}$ and $\boldsymbol{N}$ in Loc can be linked by a chain of Cauchy morphisms if and only if their Cauchy surfaces are related by an orientation-preserving diffeomorphism (see [17, Prop. 2.4], which builds on an older argument of Fulling, Narcowich and Wald [21]). The construction used is shown schematically in Fig. 2: the main point is the construction of the interpolating spacetime $\boldsymbol{I}$ that 'looks like' $\boldsymbol{N}$ in its past and $\boldsymbol{M}$ in its future. The assumption that $\mathscr{A}$ has the timeslice property entails the existence of an isomorphism between $\mathscr{A}(\boldsymbol{M})$ and $\mathscr{A}(\boldsymbol{N})$; indeed, there are many such isomorphisms, because there is considerable freedom in the choice of interpolating spacetime, none of which can be regarded as canonical.

The assumptions just stated are satisfied by simple models, such as the free Klein–Gordon field [2], and, importantly, by perturbatively constructed models of a scalar field with self-interaction [1, 26, 27]. In order to be self-contained, we briefly describe the free theory corresponding to the minimally coupled Klein–Gordon theory, with field equation $(\Box_{\boldsymbol{M}} + m^2)\phi = 0$: in each spacetime $\boldsymbol{M} \in \mathsf{Loc}$, one

defines a unital $*$-algebra $\mathscr{A}(\boldsymbol{M})$ with generators $\Phi_{\boldsymbol{M}}(f)$ ('smeared fields') labelled by test functions $f \in C_0^\infty(\boldsymbol{M})$ and subject to the following relations:

- $f \mapsto \Phi_{\boldsymbol{M}}(f)$ is linear
- $\Phi_{\boldsymbol{M}}(f)^* = \Phi_{\boldsymbol{M}}(\bar{f})$
- $\Phi_{\boldsymbol{M}}((\Box_{\boldsymbol{M}} + m^2)f) = 0$
- $[\Phi_{\boldsymbol{M}}(f), \Phi_{\boldsymbol{M}}(f')] = iE_{\boldsymbol{M}}(f,f')\mathbf{1}_{\mathscr{A}(\boldsymbol{M})}$

where

$$E_{\boldsymbol{M}}(f,f') = \int_{\boldsymbol{M}} f(p)\left((E^-_{\boldsymbol{M}} - E^+_{\boldsymbol{M}})f'\right)(p)d\mathrm{vol}_{\boldsymbol{M}}(p) \tag{4}$$

is constructed from the advanced $(-)$ and retarded $(+)$ Green operators (which obey $\mathrm{supp}\,(E^\pm_{\boldsymbol{M}}f) \subset J^\pm_{\boldsymbol{M}}(\mathrm{supp} f)$). This defines the objects of the theory; for the morphisms, any hyperbolic embedding $\psi : \boldsymbol{M} \to \boldsymbol{N}$ determines a unique morphism $\mathscr{A}(\psi) : \mathscr{A}(\boldsymbol{M}) \to \mathscr{A}(\boldsymbol{N})$ with the property

$$\mathscr{A}(\psi)\Phi_{\boldsymbol{M}}(f) = \Phi_{\boldsymbol{N}}(\psi_* f) \qquad (f \in C_0^\infty(\boldsymbol{M})), \tag{5}$$

where ψ_* is the push-forward. The proof that $\mathscr{A}(\psi)$ is well-defined as a morphism of Alg relies on the properties of globally hyperbolic spacetimes, the definition of hyperbolic embeddings, and some algebraic properties of the algebras $\mathscr{A}(\boldsymbol{M})$ [notably, that they are simple].

Our discussion will use two more features of the general structure. First, let $\mathscr{D}$ be the functor assigning test function spaces to spacetimes, $\mathscr{D}(\boldsymbol{M}) = C_0^\infty(\boldsymbol{M})$, and the push-forward to morphisms $\mathscr{D}(\psi) = \psi_*$. Then (5) precisely asserts the existence of a natural transformation Φ between the functors $\mathscr{D}$ and $\mathscr{A}$ (modulo a forgetful functor from Alg to the category of vector spaces) [2]. We take this as the prototype of what a field should be in the locally covariant setting, allowing for fields depending nonlinearly on the test function by using a forgetful functor from Alg to the category of sets, and for other tensorial types by suitable alternative choices of $\mathscr{D}$. As will be discussed later, spinorial fields require a modification of the category Loc.

Second, natural transformations may also be used to compare locally covariant theories. A natural $\eta : \mathscr{A} \dot{\to} \mathscr{B}$ is interpreted as an embedding of $\mathscr{A}$ as a subtheory of $\mathscr{B}$, while a natural isomorphism indicates that the theories are physically equivalent [2, 17]. Naturality requires that to each $\boldsymbol{M} \in \mathsf{Loc}$ there is a morphism $\eta_{\boldsymbol{M}} : \mathscr{A}(\boldsymbol{M}) \to \mathscr{B}(\boldsymbol{M})$

$$\eta_{\boldsymbol{N}} \circ \mathscr{A}(\psi) = \mathscr{B}(\psi) \circ \eta_{\boldsymbol{M}} \tag{6}$$

for each morphism $\psi : \boldsymbol{M} \to \boldsymbol{N}$. The interpretation of η as a subtheory embedding can be justified on several grounds – see [17].

The equivalences of $\mathscr{A}$ with itself form the group $\mathrm{Aut}(\mathscr{A})$ of automorphisms of the functor. This has a nice physical interpretation: it is the global gauge group [14].

Locally covariant QFT is not merely an elegant formalism for rephrasing known results and models, but has also led to new departures in the description of QFT in curved spacetimes. These can be divided into those that are model-independent and those that are specific to particular theories. Those of the former type include the spin-statistics connection [39]; the introduction of the relative Cauchy evolution and intrinsic understanding of the stress-energy tensor [2]; an analogue of the Reeh–Schlieder theorem [11, 34] and the split property [11]; new approaches to superselection theory [3, 4] and the understanding of global gauge transformations [14]; a no-go theorem for preferred states [17], and a discussion of how one can capture the idea that a theory describes 'the same physics in all spacetimes' [17]. Model-specific applications include, above all, the perturbative construction of interacting models [1, 26, 27], including those with gauge symmetries [20, 25]. However, there are also applications to the theory of Quantum Energy Inequalities [12, 16, 31] and cosmology [6, 7, 40].

3 A Rigidity Argument

The framework of local covariance appears quite loose, but in fact the descriptions of the theory in different spacetimes are surprisingly tightly related. There are various interesting properties which, if they hold in Minkowski space, must also hold in general spacetimes. This will apply in particular to the spin–statistics connection; as a warm-up, let us see how such arguments can be used in the context of Einstein causality, temporarily relaxing our assertion of this property as an axiom.

For $\boldsymbol{M} \in \mathsf{Loc}$, let $\mathcal{O}^{(2)}(\boldsymbol{M})$ be the set of ordered pairs of spacelike separated open globally hyperbolic subsets of $\boldsymbol{M}$. For any such pair $\langle O_1, O_2\rangle \in \mathcal{O}^{(2)}(\boldsymbol{M})$, let $P_{\boldsymbol{M}}(O_1, O_2)$ be true if $\mathscr{A}^{\mathrm{kin}}(\boldsymbol{M}; O_1)$ and $\mathscr{A}^{\mathrm{kin}}(\boldsymbol{M}; O_2)$ commute elementwise and false otherwise. We might say that $\mathscr{A}$ satisfies Einstein causality for $\langle O_1, O_2\rangle$. It is easily seen that there are relationships between these propositions:

R1 for all $\langle O_1, O_2\rangle \in \mathcal{O}^{(2)}(\boldsymbol{M})$,

$$P_{\boldsymbol{M}}(O_1, O_2) \iff P_{\boldsymbol{M}}(D_{\boldsymbol{M}}(O_1), D_{\boldsymbol{M}}(O_2)),$$

where $D_{\boldsymbol{M}}$ denotes the Cauchy development;

R2 given $\psi : \boldsymbol{M} \to \boldsymbol{N}$ then, for all $\langle O_1, O_2\rangle \in \mathcal{O}^{(2)}(\boldsymbol{M})$,

$$P_{\boldsymbol{M}}(O_1, O_2) \iff P_{\boldsymbol{N}}(\psi(O_1), \psi(O_2));$$

R3 for all $\langle O_1, O_2\rangle \in \mathcal{O}^{(2)}(\boldsymbol{M})$ and all $\widetilde{O}_i \in \mathcal{O}(\boldsymbol{M})$ with $\widetilde{O}_i \subset O_i$ $(i = 1, 2)$

$$P_{\boldsymbol{M}}(O_1, O_2) \implies P_{\boldsymbol{M}}(\widetilde{O}_1, \widetilde{O}_2).$$

R3 is an immediate consequence of isotony, and R1 follows from the timeslice property. Property R2 follows from the covariance property (3) of the kinematic net, which gives

$$[\mathscr{A}(\boldsymbol{N};\psi(O_1)),\mathscr{A}(\boldsymbol{N};\psi(O_2))] = \mathscr{A}(\psi)([\mathscr{A}(\boldsymbol{M};O_1),\mathscr{A}(\boldsymbol{M};O_2)]) \tag{7}$$

and the required property holds because $\mathscr{A}(\psi)$ is injective. In general, we will describe any collection of boolean-valued functions $P_{\boldsymbol{M}} : \mathcal{O}^{(2)}(\boldsymbol{M}) \to \{\mathsf{true},\mathsf{false}\}$ obeying R1–R3 (with $\boldsymbol{M}$ varying over Loc) as *rigid*.

Theorem 3.1 *Suppose $(P_{\boldsymbol{M}})_{\boldsymbol{M}\in\mathsf{Loc}}$ is rigid, and that $P_{\boldsymbol{M}}(O_1,O_2)$ holds for some $\langle O_1,O_2\rangle \in \mathcal{O}^{(2)}(\boldsymbol{M})$. Then $P_{\widetilde{\boldsymbol{M}}}(\widetilde{O}_1,\widetilde{O}_2)$ for every $\langle\widetilde{O}_1,\widetilde{O}_2\rangle \in \mathcal{O}^{(2)}(\widetilde{\boldsymbol{M}})$ in every spacetime $\widetilde{\boldsymbol{M}} \in \mathsf{Loc}$ for which either (a) the Cauchy surfaces of $\widetilde{O}_i$ are oriented diffeomorphic to those of O_i for $i = 1,2$; or (b) each component of $\widetilde{O}_1 \cup \widetilde{O}_2$ has Cauchy surface topology $\mathbb{R}^{n-1}$.*[4]

Proof The strategy for (a) is illustrated by Fig. 3, in which the wavy line indicates a sequence of spacetimes forming a deformation chain (cf. Fig. 2)

$$\widetilde{\boldsymbol{M}}|_{\widetilde{O}_1\cup\widetilde{O}_2} \xleftarrow{\widetilde{\psi}} \widetilde{\boldsymbol{L}} \xrightarrow{\widetilde{\varphi}} \boldsymbol{I} \xleftarrow{\varphi} \boldsymbol{L} \xrightarrow{\psi} \boldsymbol{M}|_{O_1\cup O_2}, \tag{8}$$

where $\psi,\widetilde{\psi},\varphi,\widetilde{\varphi}$ are Cauchy morphisms. By property R2, $P_{\boldsymbol{M}}(O_1,O_2)$ is equivalent to $P_{\boldsymbol{M}|_{O_1\cup O_2}}(O_1,O_2)$, and likewise $P_{\widetilde{\boldsymbol{M}}}(\widetilde{O}_1,\widetilde{O}_2)$ is equivalent to $P_{\widetilde{\boldsymbol{M}}|_{\widetilde{O}_1\cup\widetilde{O}_2}}(\widetilde{O}_1,\widetilde{O}_2)$. Writing L_i and I_i for the components of $\boldsymbol{L}$ and $\boldsymbol{I}$ corresponding to O_1 and O_2, and applying R1 and R2 repeatedly,

$$\begin{aligned} P_{\boldsymbol{M}|_{O_1\cup O_2}}(O_1,O_2) &\overset{R1}{\Longleftrightarrow} P_{\boldsymbol{M}|_{O_1\cup O_2}}(\psi(L_1),\psi(L_2)) \\ &\overset{R2}{\underset{\psi}{\Longleftrightarrow}} P_{\boldsymbol{L}}(L_1,L_2) \overset{R2}{\underset{\varphi}{\Longleftrightarrow}} P_{\boldsymbol{I}}(\varphi(L_1),\varphi(L_2)) \overset{R1}{\Longleftrightarrow} P_{\boldsymbol{I}}(I_1,I_2) \end{aligned} \tag{9}$$

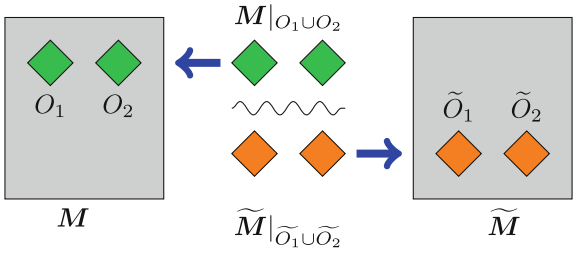


Fig. 3 Schematic representation of the rigidity argument

[4] For example, these components might be Cauchy developments of sets that are diffeomorphic to a $(n-1)$-ball and which lie in a spacelike Cauchy surface.

and in the same way, $P_{\boldsymbol{I}}(I_1, I_2)$ is also equivalent to $P_{\widetilde{\boldsymbol{M}}|_{\widetilde{O}_1 \cup \widetilde{O}_2}}(\widetilde{O}_1, \widetilde{O}_2)$. Together with the equivalences noted already, this completes the proof.

For (b), we choose, for each $i = 1, 2$, a globally hyperbolic set D_i contained in O_i and with the same number of components as $\widetilde{O}_i$, and so that all its components have Cauchy surface topology $\mathbb{R}^{n-1}$. Using R3, $P_{\boldsymbol{M}}(D_1, D_2)$, and the result follows by part (a).

As a consequence, we see that the hypothesis that Einstein causality holds in one spacetime is not independent of it holding in another. This is a prototype for the spin–statistics connection that will be described later, and is similar to the arguments used in [39]. Related arguments apply to properties such as extended locality (see [29, 37] for the original definition) and the Schlieder property (see, likewise [36]) as described in [18].

4 Framed Spacetimes

The conventional account of theories with spin is phrased in terms of spin structures. Four dimensional globally hyperbolic spacetimes support a unique spin bundle (up to equivalence) namely the trivial right-principal bundle $S\boldsymbol{M} = \boldsymbol{M} \times \mathrm{SL}(2, \mathbb{C})$ [28] and for simplicity we restrict to this situation. A spin structure σ is a double cover from $S\boldsymbol{M}$ to the frame bundle $F\boldsymbol{M}$ over $\boldsymbol{M}$ that intertwines the right-actions on $S\boldsymbol{M}$ and $F\boldsymbol{M}$: i.e., $\sigma \circ R_S = R_{\pi(S)} \circ \sigma$, where $\pi : \mathrm{SL}(2, \mathbb{C}) \to \mathcal{L}_+^\uparrow$ is the usual double cover. Pairs $(\boldsymbol{M}, \sigma)$ form the objects of a category SpinLoc, in which a morphism $\Psi : (\boldsymbol{M}, \sigma) \to (\boldsymbol{M}', \sigma')$ is a bundle morphism $\Psi : S\boldsymbol{M} \to S\boldsymbol{M}'$ which (a) covers a Loc-morphism $\psi : \boldsymbol{M} \to \boldsymbol{M}'$, i.e., $\Psi(p, S) = (\psi(p), \Xi(p)S)$ for some $\Xi \in C^\infty(\boldsymbol{M}; \mathrm{SL}(2, \mathbb{C}))$, and (b) obeys $\sigma' \circ \Psi = \psi_* \circ \sigma$, where ψ_* is the induced map of frame bundles arising from the tangent map of ψ. These structures provide the setting for the locally covariant formulation of the Dirac field [35], for instance. From an operational perspective, however, this account of spin it is not completely satisfactory, because the morphisms are described at the level of the spin bundle, to which we do not have observational access, and are only fixed up to sign by the geometric map of spacetime manifolds. To some extent, one has also introduced the understanding of spin by hand, as well, although this is reasonable enough when formulating specific models such as the Dirac field.

By contrast, the approach described here has a more operationally satisfactory basis. Instead of Loc or SpinLoc, we work on a category of *framed spacetimes* FLoc defined as follows. An object of FLoc is a pair $\mathfrak{M} = (\mathcal{M}, e)$ where $\mathcal{M}$ is a smooth manifold of fixed dimension n on which $e = (e^\nu)_{\nu=0}^{n-1}$ is a global smooth coframe (i.e., an n-tuple of smooth everywhere linearly independent 1-forms) subject to the condition that $\mathcal{M}$, equipped with the metric, orientation and time-orientation induced by e, is a spacetime in Loc, to be denoted $\mathscr{L}(\mathcal{M}, e)$. Here, the metric induced by e is $\eta_{\mu\nu} e^\mu e^\nu$, where $\eta = \mathrm{diag}(+1, -1, \ldots, -1)$, while the orientation

and time-orientation are fixed by requiring $e^0 \wedge \cdots \wedge e^{n-1}$ to be positively oriented, and e^0 to be future-directed. Similarly, a morphism $\psi : (\mathcal{M}, e) \to (\mathcal{M}', e')$ in FLoc is a smooth map between the underlying manifolds inducing a Loc-morphism $\mathscr{L}(\mathcal{M}, e) \to \mathscr{L}(\mathcal{M}', e')$ and obeying $\psi^* e' = e$. In this way, we obtain a forgetful functor $\mathscr{L} : \mathsf{FLoc} \to \mathsf{Loc}$. Moreover, FLoc is related to $\mathsf{SpinLoc}$ by a functor $\mathscr{S} : \mathsf{FLoc} \to \mathsf{SpinLoc}$ defined by

$$\mathscr{S}(\mathcal{M}, e) = (\mathscr{L}(\mathcal{M}, e), (p, S) \mapsto R_{\pi(S)} e|_p^*), \tag{10}$$

where $e|_p^*$ is the dual frame to e at p, and so that each FLoc morphism is mapped to a $\mathsf{SpinLoc}$-morphism $\mathscr{S}(\psi)$ whose underlying bundle map is $\psi \times \mathrm{id}_{\mathrm{SL}(2,\mathbb{C})}$. Essentially, $\mathscr{S}(\mathcal{M}, e)$ corresponds to the trivial spin structure associated to a frame [28], and we exploit the uniqueness of this spin structure to define the morphisms. One may easily see that $\mathscr{S}$ is a bijection on objects; however, there are morphisms in $\mathsf{SpinLoc}$ that do not have precursors in FLoc, namely, those involving local frame rotations.[5] Clearly, the composition of $\mathscr{S}$ with the obvious forgetful functor from $\mathsf{SpinLoc}$ to Loc gives the functor $\mathscr{L} : \mathsf{FLoc} \to \mathsf{Loc}$.

The description of spacetimes in Loc represents a 'rods and clocks' account of measurement.[6] However, we need to be clear that the coframe is not in itself physically significant, by contrast to the metric, orientation and time-orientation it induces. In other words, our description contains redundant information and we must take care to account for the degeneracies we have introduced. This is not a bug, but a feature: it turns out to lead to an enhanced understanding of what spin is.

In this new context, a locally covariant QFT should be a functor from FLoc to Alg (or some other category, e.g., $\mathsf{C^*\text{-}Alg}$). Of course, any theory $\mathscr{A} : \mathsf{Loc} \to \mathsf{Alg}$ induces such a functor, namely $\mathscr{A} \circ \mathscr{L} : \mathsf{FLoc} \to \mathsf{Alg}$, and likewise every $\mathscr{B} : \mathsf{SpinLoc} \to \mathsf{Alg}$ induces $\mathscr{B} \circ \mathscr{S} : \mathsf{FLoc} \to \mathsf{Alg}$, but not every theory need arise in this way. As already mentioned, we need to keep track of the redundancies in our description, namely the freedom to make *global frame rotations*. These are represented as follows. To each $\Lambda \in \mathcal{L}_+^\uparrow$, there is a functor $\mathscr{T}(\Lambda) : \mathsf{FLoc} \to \mathsf{FLoc}$

$$\mathscr{T}(\Lambda)(\mathcal{M}, e) = (\mathcal{M}, \Lambda e), \qquad \text{where } (\Lambda e)^\mu = \Lambda^\mu{}_\nu e^\nu \qquad (\Lambda \in \mathcal{L}_+^\uparrow) \tag{11}$$

with action on morphisms uniquely fixed so that $\mathscr{L} \circ \mathscr{T}(\Lambda) = \mathscr{L}$. In this way, $\Lambda \mapsto \mathscr{T}(\Lambda)$ faithfully represents $\mathcal{L}_+^\uparrow$ in $\mathrm{Aut}(\mathsf{FLoc})$. Moreover, any locally covariant

[5] Local frame rotations will appear later on, but not as morphisms.

[6] One might be concerned that the assumption that global coframes exist is restrictive, as it requires that $\mathcal{M}$ to be parallelizable. However, this presents no difficulties if $n = 4$, because all four dimensional globally hyperbolic spacetimes are parallelizable. Conceivably, one could modify the set-up in general dimensions by working with local coframes, if it was felt necessary to include non-parallelizable spacetimes.

theory $\mathscr{A}$: $\mathsf{FLoc} \to \mathsf{Alg}$ induces a family of theories

$$\mathscr{A} \circ \mathscr{T}(\Lambda) : \mathsf{FLoc} \to \mathsf{Alg} \qquad (\Lambda \in \mathcal{L}_+^{\uparrow}), \tag{12}$$

which corresponds to applying the original theory $\mathscr{A}$ to a frame-rotated version of the original spacetime. If we are to take seriously the idea that frame rotations of this type carry no physical significance then these theories should be equivalent. We formalise this in the following

Axiom 4.1 (Independence of global frame rotations) To each $\Lambda \in \mathcal{L}_+^{\uparrow}$, there exists an equivalence $\eta(\Lambda) : \mathscr{A} \dot{\to} \mathscr{A} \circ \mathscr{T}(\Lambda)$, such that

$$\eta(\Lambda)_{(\mathcal{M},e)}\alpha_{(\mathcal{M},e)} = \alpha_{(\mathcal{M},\Lambda e)}\eta(\Lambda)_{(\mathcal{M},e)} \qquad (\forall \alpha \in \mathrm{Aut}(\mathscr{A})). \tag{13}$$

The condition (13) asserts that the equivalence implementing independence of global frame rotations intertwines the action of global gauge transformations. Plausibly it might be relaxed (or modified) but it gives the cleanest results, so will be maintained for now. Note that the equivalences $\eta(\Lambda)$ are not specified beyond this requirement; what is important is that they exist. Obviously every theory induced from Loc (i.e., $\mathscr{A} = \mathscr{B} \circ \mathscr{L}$, for some $\mathscr{B} : \mathsf{Loc} \to \mathsf{Alg}$) obeys Axiom 4.1, simply by taking $\eta(\Lambda)$ to be the identity automorphism of $\mathscr{A}$.

The assumptions above have a number of consequences [10]. First, the $\eta(\Lambda)$ induce a 2-cocycle of $\mathcal{L}_+^{\uparrow}$, taking values in the centre of the global gauge group $\mathcal{Z}(\mathrm{Aut}(\mathscr{A}))$, and given by

$$\xi(\Lambda', \Lambda)_{(\mathcal{M},e)} = \eta(\Lambda)^{-1}_{(\mathcal{M},e)}\eta(\Lambda')^{-1}_{(\mathcal{M},\Lambda e)}\eta(\Lambda'\Lambda)_{(\mathcal{M},e)}; \tag{14}$$

furthermore, any other system of equivalences $\widetilde{\eta}(\Lambda) : \mathscr{A} \dot{\to} \mathscr{A} \circ \mathscr{T}(\Lambda)$ obeying (13) determines an equivalent 2-cocycle. We conclude that each theory $\mathscr{A} : \mathsf{FLoc} \to \mathsf{Alg}$ obeying Axiom 4.1 determines a group cohomology class $[\xi] \in H^2(\mathcal{L}_+^{\uparrow}; \mathcal{Z}(\mathrm{Aut}(\mathscr{A})))$ in a canonical fashion.

It is worth pausing to consider some sufficient conditions for $[\xi]$ to be trivial. This occurs, for instance, whenever $\mathscr{A}$ is induced from a theory on Loc, because we *may* take $\eta(\Lambda) = \mathrm{id}_{\mathscr{A}}$, giving $\xi(\Lambda, \Lambda') = \mathrm{id}_{\mathscr{A}}$, and any other choice gives a cohomologous 2-cocycle. Again, if $\mathscr{A}$ has global gauge group with trivial centre, then ξ has no choice but to be trivial.

Next, the *scalar* fields of the theory form a vector space $\mathrm{Fld}(\mathscr{A})$ carrying an action of both the gauge group

$$(\alpha \cdot \Phi)_{(\mathcal{M},e)}(f) = \alpha_{(\mathcal{M},e)}\Phi_{(\mathcal{M},e)}(f) \qquad (\alpha \in \mathrm{Aut}(\mathscr{A})) \tag{15}$$

and the proper orthochronous Lorentz group $\mathcal{L}_+^\uparrow$

$$(\Lambda \star \Phi)_{(\mathcal{M},\Lambda e)}(f) = \eta(\Lambda)_{(\mathcal{M},e)}\Phi_{(\mathcal{M},e)}(f) \qquad (\Lambda \in \mathcal{L}_+^\uparrow). \tag{16}$$

These two actions commute, and turn out to obey

$$(\Lambda'\Lambda) \star \Phi = \xi(\Lambda', \Lambda) \cdot (\Lambda' \star (\Lambda \star \Phi)), \tag{17}$$

which entails that irreducible subspaces of $\mathrm{Fld}(\mathscr{A})$ under the action of $\mathcal{L}_+^\uparrow \times \mathrm{Aut}(\mathscr{A})$ carry multiplier representations of $\mathcal{L}_+^\uparrow$, determined by ξ. We deduce that the scalar fields form Lorentz and gauge multiplets (extending a result on gauge multiplets from [14]). Further, all multiplets in which the multiplier representation is continuous (at least near the identity) must arise from *true* real linear representations of the covering group $\mathrm{SL}(2,\mathbb{C})$, and are therefore classified in the familiar way by pairs (j,k) where j,k are integer or half-integer spins. Accordingly our analysis has led to an emergent understanding of spin, and answers the question of why this is an appropriate physical notion in curved spacetimes.

In certain cases, we may say more immediately. Any theory induced from Loc, or in which $\mathcal{Z}(\mathrm{Aut}(\mathscr{A}))$ is trivial, can only support fields of integer-spin, because $[\xi]$ is trivial. Similarly, all multiplets of observable fields are of integer spin, because ξ is a global gauge transformation, and therefore acts trivially on such fields.

It seems remarkable that so much can be extracted from the single Axiom 4.1, without the need to specify what the equivalences $\eta(\Lambda)$ actually are. In order to prove the spin-statistics connection, however, it is convenient to be a bit more specific, and to connect them to dynamics. This requires a generalization of the spacetime deformation techniques to FLoc [10].

With this in mind, let us define FLoc-Cauchy morphisms to be FLoc morphisms ψ whose image $\mathscr{L}(\psi)$ in Loc is Cauchy according to our earlier definition. Further, let us assume that $\mathscr{A} : \mathsf{FLoc} \to \mathsf{Alg}$ has the timeslice property and so maps any FLoc-Cauchy morphism to an isomorphism in Alg. Fixing $(\mathcal{M}, e) \in \mathsf{FLoc}$, any $\widetilde{\Lambda} \in C^\infty(\mathcal{M}; \mathcal{L}_+^\uparrow)$ that is trivial outside a time-compact set[7] induces a relative Cauchy evolution, illustrated in Fig. 4, and given by

$$\mathrm{rce}_{(\mathcal{M},e)}[\widetilde{\Lambda}] = \mathscr{A}(\iota^-) \circ \mathscr{A}(\iota^-[\widetilde{\Lambda}])^{-1} \circ \mathscr{A}(\iota^+[\widetilde{\Lambda}]) \circ \mathscr{A}(\iota^+)^{-1}. \tag{18}$$

However, it would seem strange if such a frame rotation could induce physical effects in the overall evolution. Taking a more conservative stance, let us weaken that to cover only those frame rotations that can be deformed away homotopically. It seems reasonable to posit:

[7] That is, a set that lies to the future of one Cauchy surface and the past of another.

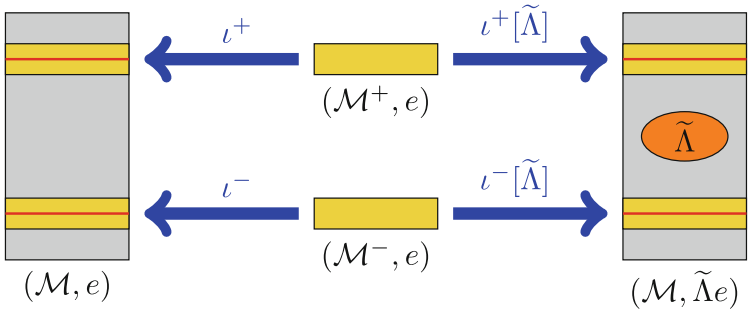


Fig. 4 Schematic representation of the relative Cauchy evolution induced by a local frame rotation

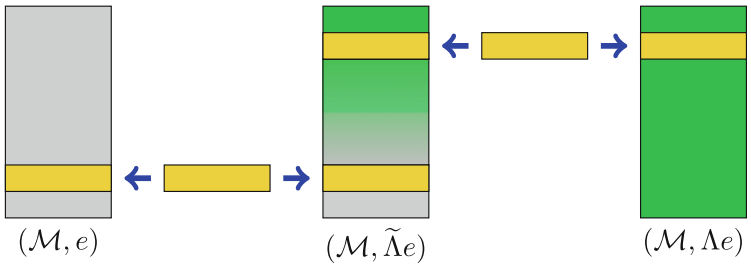


Fig. 5 Construction of the natural transformations $\zeta(S)$

Axiom 4.2 (Independence of local frame rotations) $\mathrm{rce}_{(\mathcal{M},e)}[\widetilde{\Lambda}] = \mathrm{id}_{\mathscr{A}(\mathcal{M},e)}$ for homotopically trivial $\widetilde{\Lambda}$.

Axiom 4.2 has an important consequence. Consider the chain of spacetimes illustrated in Fig. 5, in which the morphisms illustrated are all Cauchy, and $\widetilde{\Lambda} \in C^\infty(\mathcal{M}; \mathcal{L}_+^\uparrow)$ is equal to the identity in the past region and takes the constant value Λ in the future region. Then the timeslice axiom induces an isomorphism $\mathscr{A}(\mathcal{M}, e) \to \mathscr{A}(\mathcal{M}, \Lambda e)$. Crucially, Axiom 4.2 entails that the isomorphism depends on $\widetilde{\Lambda}$ only via its homotopy class. Thus each S in the universal cover $\widetilde{\mathcal{L}_+^\uparrow}$ of $\mathcal{L}_+^\uparrow$ induces isomorphisms

$$\zeta_{(\mathcal{M},e)}(S) : \mathscr{A}(\mathcal{M}, e) \longrightarrow \mathscr{A}(\mathcal{M}, \pi(S)e). \tag{19}$$

Let us assume (although one might suspect this can be *derived*) that the $\zeta_{(\mathcal{M},e)}(S)$ cohere to give natural isomorphisms

$$\zeta(S) : \mathscr{A} \dot{\to} \mathscr{A} \circ \mathscr{T}(\pi(S)). \tag{20}$$

We may now replicate our previous analysis, with $S \mapsto \zeta(S)$ in place of $\Lambda \mapsto \eta(\Lambda)$, leading to a 2-cocycle of the universal cover of $\mathcal{L}_+^\uparrow$ in $\mathrm{Aut}(\mathscr{A})$ that is trivial; indeed, one may show that

$$\zeta(S')_{(\mathcal{M},\pi(S)e)}\zeta(S)_{(\mathcal{M},e)} = \zeta(S'S)_{(\mathcal{M},e)} \qquad (S, S' \in \mathcal{L}_+^\uparrow).$$

In $n = 4$ dimensions, we note that $\zeta(-1)$ is an automorphism of $\mathscr{A}$ (as $\pi(-1) = 1$); moreover, it obeys

$$\zeta(-1)^2 = \zeta(1) = \mathrm{id}, \tag{21}$$

which one might think of as a spacetime version of Dirac's belt trick.

It is important to connect our discussion of frame rotations with the familiar implementation of the Lorentz group in Minkowski space. In our present setting, n-dimensional Minkowski space is the object $\mathfrak{M}_0 = (\mathbb{R}^n, (dX^\mu)_{\mu=0}^{n-1})$, where $X^\mu : \mathbb{R}^n \to \mathbb{R}$ are the standard coordinate functions $X^\mu(x^0, \ldots, x^{n-1}) = x^\mu$. Any $\Lambda \in \mathcal{L}_+^\uparrow$ induces an active Lorentz transformation $\Lambda : \mathbb{R}^n \to \mathbb{R}^n$ by matrix multiplication, $X^\mu \circ \Lambda = \Lambda^\mu{}_\nu X^\nu$, which induces a morphism

$$\psi_\Lambda : \mathfrak{M}_0 \to \mathscr{T}(\Lambda^{-1})(\mathfrak{M}_0) \tag{22}$$

in FLoc. One may verify that $\psi_{\Lambda'\Lambda} = \mathscr{T}(\widetilde{\Lambda^{-1}})(\psi_{\Lambda'}) \circ \psi_\Lambda$. Accordingly, we obtain an automorphism of $\mathscr{A}(\mathfrak{M}_0)$ for each $S \in \widetilde{\mathcal{L}_+^\uparrow}$ by

$$\Xi(S) = \zeta(S)_{\mathscr{T}(\pi(S)^{-1})(\mathfrak{M}_0)} \circ \mathscr{A}(\psi_{\pi(S)}). \tag{23}$$

It may be checked that $\Xi(S'S) = \Xi(S') \circ \Xi(S)$ and that one has

$$\Xi(S)\Phi_{\mathfrak{M}_0}(f) = (S \star \Phi)_{\mathfrak{M}_0}(\pi(S)_* f) \qquad (f \in C_0^\infty(\mathbb{R}^n)), \tag{24}$$

where we now extend the action on fields from the Lorentz group to its universal cover. In particular, for $n = 4$, any 2π-rotation corresponds to

$$\Xi(-1) = \zeta(-1)_{\mathfrak{M}_0}. \tag{25}$$

Given a state ω_0 on $\mathscr{A}(\mathfrak{M}_0)$ that is invariant under the automorphisms, i.e., $\omega_0 \circ \Xi(S) = \omega_0$ for all S, the corresponding GNS representation will carry a unitary implementation of the $\Xi(S)$, which recovers the standard formulation.

5 Spin and Statistics in Four Dimensions

We come to the proof of the spin–statistics connection [10]. As in [39], the idea is to refer the statement in a general spacetime back to Minkowski space, where standard spin–statistics results can be applied. In other words, we apply a rigidity argument. The notion of statistics employed is based on graded commutativity of local algebras at spacelike separation.

Definition 5.1 An involutory global gauge transformation $\gamma \in \mathrm{Aut}(\mathscr{A})$, $\gamma^2 = \mathrm{id}$ is said to *grade statistics* in $\mathfrak{M}$ if, for all spacelike separated regions $O_i \in \mathcal{O}(\mathfrak{M})$, every component of which has Cauchy surface topology $\mathbb{R}^3$, one has

$$A_1 A_2 = (-1)^{\sigma_1 \sigma_2} A_2 A_1 \tag{26}$$

for all $A_i \in \mathscr{A}^{\mathrm{kin}}(\mathfrak{M}; O_i)$ s.t., $\gamma_{\mathfrak{M}} A_i = (-1)^{\sigma_i} A_i$.

The standard spin–statistics connection, in view of (25), asserts that $\zeta(-1)$ grades statistics in Minkowski space $\mathfrak{M}_0$, where $\zeta(S)$ is defined as in Sect. 4.

Theorem 5.2 *If γ grades statistics in $\mathfrak{M}_0$, then it does so in every spacetime of* FLoc*. Consequently, if the theory obeys the standard spin–statistics connection in Minkowski space, $\zeta(-1)$ grades statistics on every framed spacetime $\mathfrak{M} \in$ FLoc.*

Proof (Sketch) For each $\langle O_1, O_2 \rangle \in \mathcal{O}^{(2)}(\boldsymbol{M})$, let $P_{\mathfrak{M}}(O_1, O_2)$ be the statement that

$$A_1 A_2 = (-1)^{\sigma_1 \sigma_2} A_2 A_1 \text{ for all } A_i \in \mathscr{A}^{\mathrm{kin}}(\mathfrak{M}; O_i) \text{ s.t., } \gamma_{\mathfrak{M}} A_i = (-1)^{\sigma_i} A_i. \tag{27}$$

We argue that the collection $(P_{\mathfrak{M}})_{\mathfrak{M} \in \mathsf{FLoc}}$ is rigid, whereupon the result holds by a generalization of Theorem 3.1 to FLoc. R1 and R3 hold for the same reasons used in Sect. 3 for Einstein causality. For R2, we note that the subspaces

$$\mathscr{A}^{\mathrm{kin}}_{\sigma}(\mathfrak{M}; O) = \{A \in \mathscr{A}^{\mathrm{kin}}(\mathfrak{M}; O) : \gamma_{\mathfrak{M}} A = (-1)^{\sigma} A\} \qquad \sigma \in \{0, 1\} \tag{28}$$

obey, for any $\psi : \mathfrak{M} \to \widetilde{\mathfrak{M}}$,

$$\mathscr{A}^{\mathrm{kin}}_{\sigma}(\widetilde{\mathfrak{M}}; \psi(O)) = \mathscr{A}(\psi)(\mathscr{A}^{\mathrm{kin}}_{\sigma}(\mathfrak{M}; O)) \tag{29}$$

by naturality of γ and injectivity of $\mathscr{A}(\psi)$. A further use of injectivity gives

$$P_{\widetilde{\mathfrak{M}}}(\psi(O_1), \psi(O_2)) \iff P_{\mathfrak{M}}(O_1, O_2), \tag{30}$$

thus establishing R2 and concluding the proof.

What is really being proved is the connection between the statistics grading in Minkowski space and that in arbitrary spacetimes. Thus, a locally covariant theory that violates the standard spin-statistics connection in Minkowski space (e.g., a ghost theory) but in which the statistics grading is still implemented (in

Minkowski) by an involutory gauge transformation, would be covered by our result – the statistics would be consistently graded in all spacetimes by the same gauge transformation.

6 Summary and Outlook

The BFV paper [2] is subtitled 'A new paradigm for local quantum physics', and indeed their paper marked the beginnings of a full development of a model-independent account of QFT in CST, the current state of which is described in more detail in [18]. At the heart of this approach is the fact that local covariance is a surprisingly rigid structure, which makes it possible to transfer certain results from the flat spacetime situation into general curved spacetimes in a fairly systematic way. This is a consequence of the timeslice property and also the structure of the categories Loc and FLoc.

In this contribution, I have focussed particularly on the spin-statistics connection, which was one of the starting points for the general theory. I have described a new viewpoint, based on framed spacetimes, that gives a more operational starting point for the discussion of spin in locally covariant QFT, without making reference to unobservable geometric structures such as spin bundles. Instead, by recognizing that we make physical measurements using frames, and by tracking the concomitant redundancies, we are led naturally to a description that allows for spin. In our discussion, the relative Cauchy evolution, which plays an important role in locally covariant physics on Loc, is developed further so as to cater for deformation of the framing, rather than just of the metric.

Certain issues remain to be understood. Our view of statistics has focussed on graded commutativity at spacelike separation; it is not currently clear how to make contact with the occurrence of braid statistics in low dimensions. The coframed spacetimes we consider are necessarily parallelizable; while this is not a restriction in four spacetime dimensions, one could seek generalizations that accommodate nonparallelizable spacetimes of other dimensions. Finally, neither the result described here, nor Verch's result [39], gives a direct proof of the spin-statistics connection in curved spacetime; both rely on the classic results of Minkowski space QFT. Now a proof is a proof, and perhaps one should not complain too much, because it may be that a direct argument would be considerably more involved than those we now have. Nonetheless, arguments that provide more insight into the nature of the spin-statistics connection are still desirable and it is hoped that the more operational account of spin presented here can be a further step along that path.

Acknowledgements I thank the organisers and participants of the *Quantum Mathematical Physics* conference in Regensburg (2014) for their interest and comments, and also the various sponsoring organizations of the meeting for financial support.

References

1. R. Brunetti, K. Fredenhagen, Microlocal analysis and interacting quantum field theories: renormalization on physical backgrounds. Commun. Math. Phys. **208**, 623–661 (2000)
2. R. Brunetti, K. Fredenhagen, R. Verch, The generally covariant locality principle: a new paradigm for local quantum physics. Commun. Math. Phys. **237**, 31–68 (2003). math-ph/0112041
3. R. Brunetti, G. Ruzzi, Superselection sectors and general covariance. I. Commun. Math. Phys. **270**, 69–108 (2007). gr-qc/0511118.
4. R. Brunetti, G. Ruzzi, Quantum charges and spacetime topology: the emergence of new superselection sectors. Commun. Math. Phys. **287**, 523–563 (2009)
5. N. Burgoyne, On the connection of spin with statistics. Nuovo Cimento **10**(8), 607–609 (1958)
6. C. Dappiaggi, K. Fredenhagen, N. Pinamonti, Stable cosmological models driven by a free quantum scalar field. Phys. Rev. **D77**, 104015 (2008). arXiv:0801.2850
7. A. Degner, R. Verch, Cosmological particle creation in states of low energy. J. Math. Phys. **51**, 022302 (2010)
8. S. Doplicher, R. Haag, J.E. Roberts, Local observables and particle statistics. II. Commun. Math. Phys. **35**, 49–85 (1974)
9. H. Epstein, CTP invariance of the S-matrix in a theory of local observables. J. Math. Phys. **8**, 750–767 (1967)
10. C.J. Fewster, The spin–statistics connection in curved spacetimes (In preparation)
11. C.J. Fewster, The split property for locally covariant quantum field theories in curved spacetime. ArXiv:1501.02682
12. C.J. Fewster, Quantum energy inequalities and local covariance. II. Categorical formulation. Gen. Relativ. Gravit. **39**, 1855–1890 (2007)
13. C.J. Fewster, On the notion of 'the same physics in all spacetimes', in *Quantum Field Theory and Gravity. Conceptual and Mathematical Advances in the Search for a Unified Framework*, ed. by F. Finster, O. Müller, M. Nardmann, J. Tolksdorf, E. Zeidler (Birkhäuser, Basel, 2012), pp. 207–227. arXiv:1105.6202
14. C.J. Fewster, Endomorphisms and automorphisms of locally covariant quantum field theories. Rev. Math. Phys. **25**, 1350008, 47 (2013). arXiv:1201.3295
15. C.J. Fewster, Locally covariant quantum field theory and the problem of formulating the same physics in all spacetimes. Phil. Trans. A. Roy. Soc. (2015) arXiv:1502.04642 (To appear)
16. C.J. Fewster, M.J. Pfenning, Quantum energy inequalities and local covariance. I: globally hyperbolic spacetimes. J. Math. Phys. **47**, 082303 (2006). math-ph/0602042
17. C.J. Fewster, R. Verch, Dynamical locality and covariance: what makes a physical theory the same in all spacetimes? Ann. H. Poincaré **13**, 1613–1674 (2012). arXiv:1106.4785
18. C.J. Fewster, R. Verch, *Algebraic Quantum Field Theory in Curved Spacetimes* (2015). ArXiv:1504.00586
19. M. Fierz, Über die relativistische Theorie kräftefreier Teilchen mit beliebigem Spin. Helv. Phys. Acta **12**, 3–37 (1939)
20. K. Fredenhagen, K. Rejzner, Batalin-Vilkovisky formalism in perturbative algebraic quantum field theory. Commun. Math. Phys. **317**, 697–725 (2013)
21. S.A. Fulling, F.J. Narcowich, R.M. Wald, Singularity structure of the two-point function in quantum field theory in curved spacetime. II. Ann. Phys. **136**, 243–272 (1981)
22. D. Guido, R. Longo, An algebraic spin and statistics theorem. Commun. Math. Phys. **172**, 517–533 (1995)
23. R. Haag, *Local Quantum Physics: Fields, Particles, Algebras* (Springer, Berlin, 1992)
24. A. Higuchi, L. Parker, Y. Wang, Consistency of Faddeev-Popov ghost statistics with gravitationally induced pair creation. Phys. Rev. D **42**, 4078–4081 (1990)
25. S. Hollands, Renormalized quantum Yang-Mills fields in curved spacetime. Rev. Math. Phys. **20**, 1033–1172 (2008)

26. S. Hollands, R.M. Wald, Local Wick polynomials and time ordered products of quantum fields in curved spacetime. Commun. Math. Phys. **223**, 289–326 (2001). gr-qc/0103074
27. S. Hollands, R.M. Wald, Existence of local covariant time ordered products of quantum fields in curved spacetime. Commun. Math. Phys. **231**, 309–345 (2002). gr-qc/0111108.
28. C.J. Isham, Spinor fields in four-dimensional space-time. Proc. R. Soc. Lond. Ser. A **364**, 591–599 (1978)
29. L.J. Landau, A note on extended locality. Commun. Math. Phys. **13**, 246–253 (1969)
30. G. Lüders, B. Zumino, Connection between spin and statistics. Phys. Rev. **110**(2), 1450–1453 (1958)
31. P. Marecki, Bounds on the energy densities of ground states on static spacetimes of compact objects. Phys. Rev. D **73**, 124009 (2006). gr-qc/0507089
32. L. Parker, Y. Wang, Statistics from dynamics in curved spacetime. Phys. Rev. D **39**, 3596–3605 (1989)
33. W. Pauli, The connection between spin and statistics. Phys. Rev. **58**, 716–722 (1940)
34. K. Sanders, On the Reeh-Schlieder property in curved spacetime. Commun. Math. Phys. **288**, 271–285 (2009)
35. K. Sanders, The locally covariant Dirac field. Rev. Math. Phys. **22**, 381–430 (2010)
36. S. Schlieder, Einige Bemerkungen über Projektionsoperatoren (Konsequenzen eines Theorems von Borchers). Commun. Math. Phys. **13**, 216–225 (1969)
37. A. Schoch, On the simplicity of Haag fields. Int. J. Theor. Phys. **1**, 107–113 (1968)
38. R.F. Streater, A. S. Wightman, *PCT, spin and statistics, and all that*. Corrected third printing of the 1978 edition (Princeton Landmarks in Physics Princeton University Press, Princeton, 2000)
39. R. Verch, A spin-statistics theorem for quantum fields on curved spacetime manifolds in a generally covariant framework. Commun. Math. Phys. **223**, 261–288 (2001). math-ph/0102035
40. R. Verch, Local covariance, renormalization ambiguity, and local thermal equilibrium in cosmology, in *Quantum Field Theory and Gravity. Conceptual and Mathematical Advances in the Search for a Unified Framework*, ed. by F. Finster, O. Müller, M. Nardmann, J. Tolksdorf, E. Zeidler (Birkhäuser, Basel, 2012), pp. 229–256. arXiv:1105.6249
41. R.M. Wald, Existence of the S-matrix in quantum field theory in curved space-time. Ann. Phys. **118**, 490–510 (1979)

Is There a *C*-Function in 4D Quantum Einstein Gravity?

Daniel Becker and Martin Reuter

Contents

Abstract We describe a functional renormalization group-based method to search for '*C*-like' functions with properties similar to that in 2D conformal field theory. It exploits the mode counting properties of the effective average action and is particularly suited for theories including quantized gravity. The viability of the approach is demonstrated explicitly in a truncation of 4 dimensional Quantum Einstein Gravity, i.e. asymptotically safe metric gravity.

Keywords Quantum gravity • Asymptotic safety • *c*-theorem.

Mathematics Subject Classification (2010). Primary 81T06; Secondary 81Q06.

D. Becker (✉) • M. Reuter
Institute of Physics, University of Mainz, Staudingerweg 7, D-55099 Mainz, Germany
e-mail: BeckerD@thep.physik.uni-mainz.de; Reuter@thep.physik.uni-mainz.de

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_2

1 Introduction

A particularly intriguing result in 2-dimensional conformal field theory is Zamolodchikov's c-theorem [1]. It states that every 2D Euclidean quantum field theory with reflection positivity, rotational invariance, and a conserved energy momentum tensor possesses a function C of its coupling constants, which is non-increasing along the renormalization group trajectories and is stationary at fixed points where it equals the central charge of the corresponding conformal field theory. After the advent of this theorem many authors tried to find a generalization that would be valid also in dimensions greater than two [2–9]. This includes, for instance, suggestions by Cardy [2] to integrate the trace anomaly of the energy-momentum tensor $\langle T_{\mu\nu}\rangle$ over a 4-sphere of unit radius, $C \propto \int_{S^4} \mathrm{d}^4x\sqrt{g}\,\langle T^\mu_\mu\rangle$, the work of Osborn [3], and ideas based on the similarity of C to the thermodynamical free energy [4], leading to a conjectural 'F-theorem' which states that, under certain conditions, the finite part of the free energy of 3-dimensional field theories on S^3 decreases along renormalization group (RG) trajectories and is stationary at criticality [5]. Cappelli, Friedan and Latorre [6] proposed to define a C-function on the basis of the spectral representation of the 2-point function of the energy-momentum tensor. While these investigations led to many important insights into the expected structure of the hypothetical higher-dimensional C-function, the search was successful only recently [10, 11] with the proof of the 'a-theorem' [2, 9]. According to the a-theorem, the coefficient of the Euler form term in the induced gravity action of a 4D theory in a curved, but classical, background spacetime is non-increasing along RG-trajectories. Clearly theorems of this type are extremely valuable as they provide non-perturbative information about quantum field theories or statistical systems in the strong coupling domain and constrain the structure of possible RG flows.

In this article we are going to describe a functional RG-based search strategy by means of which 'C-like' functions can possibly be identified under rather general conditions, in particular in cases where the known c- and the a-theorems do not apply. Our main motivation is in fact theories which include quantized gravity, in particular those based upon the Asymptotic Safety construction [12–19].

According to this strategy, the first step consists in trying to generalize the 'counting property' of Zamolodchikov's C-function for a generic field theory in any number of dimensions: the sought-after function should roughly be equal to (or at least in a known way be related to) the number of degrees of freedom that are integrated out along the RG trajectory when the scale is lowered from the ultraviolet (UV) towards the infrared (IR). Technically, we shall do this by introducing a higher-derivative mode-suppression factor in the underlying functional integral which acts as an IR cutoff. We can then take advantage of the well established framework of the effective average action (EAA) to control the scale dependence [20], and to give a well defined meaning to the notion of a 'number of modes'.

In a generic theory comprising a set of dynamical fields, Φ, and associated background fields, $\bar{\Phi}$, the EAA is a 'running' functional $\Gamma_k[\Phi, \bar{\Phi}]$ similar to the standard effective action, but with a built-in IR cutoff at a variable mass scale

k. Its k-dependence is governed by an exact functional RG equation (FRGE). In this article we shall argue that there exists a natural and 'essentially universal' map from k-dependent functionals Γ_k to functions $\mathscr{C}_k$ that are monotone along the flow and stationary at fixed points. Here the term 'universal' is to indicate that we would require only a few general properties to be satisfied, comparable to reflection positivity, rotational invariance, etc. in the case of Zamolodchikov's theorem. The reason why we believe that there should exist such a map is that the respective monotonicity properties of Γ_k and the C-function in 2D have essentially the same simple origin. They both 'count' in a certain way the degrees of freedom (more precisely: fluctuation modes) that are already integrated out at a given RG scale intermediate between the UV and the IR.

After a brief review of the necessary EAA apparatus, we shall present a promising candidate for a quantity with properties close to a C-function. It is obtained by evaluating $\Gamma_k[\Phi, \bar{\Phi}]$ at a particularly chosen pair of *k-dependent* arguments $(\Phi, \bar{\Phi})$, namely $\Phi = \bar{\Phi} \equiv \bar{\Phi}_k^{\rm sc}$ where $\bar{\Phi}_k^{\rm sc}$ is a *self-consistent background field*. By definition, $\bar{\Phi} \equiv \bar{\Phi}_k^{\rm sc}$ is self-consistent ('sc') if the equation of motion for the dynamical field Φ derived from Γ_k admits the solution $\Phi = \bar{\Phi}$. With other words, if the system is put in a background which is self-consistent, the fluctuations of the dynamical field, $\varphi \equiv \Phi - \bar{\Phi}$, have zero expectation value and, in this sense, do not modify this special background. As we shall see, in theories without fermions, $\mathscr{C}_k \equiv \Gamma_k[\bar{\Phi}_k^{\rm sc}, \bar{\Phi}_k^{\rm sc}]$ has indeed a number of attractive properties making it almost a C-function. It is stationary at fixed points and it is monotonically decreasing along the flow, at least when split-symmetry is broken only sufficiently weakly.

The latter restriction is crucial and requires an explanation. In quantum gravity, Background Independence is a central requirement [21] which, in the EAA framework, is met by employing the background field technique. At the intermediate steps of the quantization one introduces a background spacetime, equipped with a non-degenerate background metric in particular, but makes sure that no observable prediction depends on it. This can be done by means of the Ward identities pertaining to the split-symmetry [22–24] which governs the interrelation between φ and $\bar{\Phi}$. This symmetry, if intact, ensures that the physical contents of a theory is independent of the chosen background structures. Usually, at the 'off-shell' level of Γ_k, in particular when $k > 0$, the symmetry is broken by the gauge fixing and cutoff terms in the bare action. Insisting on unbroken split-symmetry in the physical sector restricts the admissible RG trajectories which the EAA may follow [25, 26]; only those which restore perfect split-symmetry at their end point ($k = 0$) are acceptable. The 'sufficiently weak split-symmetry breaking' mentioned above is a related, but not exactly the same requirement, namely that the amount of symmetry breaking, on all scales $k \geq 0$, does not exceed a certain bound (given by Eq. (36) below).

Specifically we shall apply these ideas within the Asymptotic Safety approach to quantum gravity in the following [12–19]. The goal of the Asymptotic Safety program is to precisely define, and then to actually compute functional integrals over 'all metrics' such as $\int \mathcal{D}\hat{g}\, e^{-S[\hat{g}_{\mu\nu}]}$. The idea is to proceed indirectly and reconstruct the integral from a solution of the FRGE for the EAA. Contrary to the functional integral, the FRGE is free from any UV singularities. The nontrivial issue

then consists in finding an RG trajectory consisting of *regular* action functionals $\{\Gamma_k[\,\cdot\,]\}$ that is *complete*, i.e. has well defined limits $k \to 0$ and $k \to \infty$, respectively. Asymptotic Safety is a property that ensures the existence of the UV limit, $k \to \infty$. Its prerequisite is a fixed point of the RG flow, Γ_*. Let us assume there exists such a fixed point, and let $\mathscr{S}_{\rm UV}$ denote its UV critical manifold, that is the set of all actions which are pulled into Γ_* under the inverse flow (i.e. when going from the IR to the UV). Then, for the $k \to \infty$ limit to exist it is sufficient (and probably also necessary) to select any of the trajectories inside $\mathscr{S}_{\rm UV}$; we can then be sure that it has a singularity free UV behavior since it will always run into the fixed point at large scales and is easy to control then.

The only free choice in this entire construction concerns the *theory space*, $\mathcal{T}$, i.e. the space of functionals on which the FRGE operates; in particular the fields the functionals depend on, and their symmetries must be specified. Given $\mathcal{T}$, the form of the FRGE and so ultimately also its fixed point properties are determined. As $\Gamma_{k\to\infty}$ is closely related to the bare action S, we are actually *computing* S from the fixed point condition, rather than putting it in 'by hand'. Knowing Γ_* and the RG flow in its vicinity, and selecting an UV regularization scheme for the functional integral, one can in principle compute how the bare parameters on which this integral depends must be tuned in order to obtain a well defined limit when its UV regulator is removed, or the 'continuum limit' is taken [27]. For further details on Asymptotic Safety and the status of the program we refer to the reviews [17–19].

The rest of this article is organized as follows. In Sect. 2 we explain how the EAA can be used in order to 'count' field modes, and we identify a natural candidate for a 'C-function like' quantity that exists in any number of dimensions. In Sect. 3 we apply these ideas to asymptotically safe metric gravity, or 'Quantum Einstein Gravity' (QEG), and Sect. 4 contains the conclusions.

Our presentation follows Ref. [28] to which the reader is referred for additional details.

2 From the EAA to the $\mathscr{C}$-Function

We consider a general quantum field theory on a d dimensional Euclidean spacetime, either rigid or fluctuating, that is governed by a functional integral $Z = \int \mathcal{D}\hat{\Phi}\, e^{-S[\hat{\Phi},\bar{\Phi}]}$. The bare action S depends on a set of commuting and anticommuting dynamical fields, $\hat{\Phi}$, and on a corresponding set of background fields, $\bar{\Phi}$. In a Yang-Mills theory, $\hat{\Phi}$ would contain both the gauge field and the Faddeev-Popov ghosts, and S includes gauge fixing and ghost terms. Furthermore, the corresponding background fields are part of $\bar{\Phi}$. As a rule, the *fluctuation field* $\hat{\varphi} \equiv \hat{\Phi} - \bar{\Phi}$ is always required to gauge-transform homogeneously, i.e. like a matter field. Henceforth we regard $\hat{\varphi}$ rather than $\hat{\Phi}$ as the true dynamical variable and interpret Z as an integral over the fluctuation variables: $Z = \int \mathcal{D}\hat{\varphi}\, \exp\big(-S[\hat{\varphi};\bar{\Phi}]\big)$.

The set of background fields, $\bar{\Phi}$, always contains a classical spacetime metric $\bar{g}_{\mu\nu}$. In typical particle physics applications on a rigid spacetime one is not interested in how Z depends on this background metric and usually sets $\bar{g}_{\mu\nu} = \delta_{\mu\nu}$ throughout. Here in quantum gravity, where Background Independence is an issue, one needs to know $Z \equiv Z[\bar{g}_{\mu\nu}]$ for *any* background. In fact, employing the background field technique to implement Background Independence one represents the dynamical metric as $\hat{g}_{\mu\nu} = \bar{g}_{\mu\nu} + \hat{h}_{\mu\nu}$ and requires invariance under split-symmetry transformations $\left(\delta\bar{g}_{\mu\nu} = -\varepsilon_{\mu\nu},\, \delta\hat{h}_{\mu\nu} = \varepsilon_{\mu\nu}\right)$ at the level of observable quantities [25]. Assuming in the sequel that spacetime is dynamical, $\hat{g}_{\mu\nu}$ and $\hat{h}_{\mu\nu}$ are special components of $\hat{\Phi}$ and $\hat{\varphi}$, respectively.

Picking a basis in field space, $\{\varphi_\omega\}$, we expand $\hat{\varphi}(x) = \sum_\omega a_\omega\, \varphi_\omega(x)$, where $\sum_\omega$ stands for a summation and/or integration over all labels carried by the basis elements. Then $\int \mathcal{D}\hat{\varphi}$ is interpreted as the integration over all possible values that can be assumed by the expansion coefficients $a \equiv \{a_\omega\}$. Thus, $Z = \prod_\omega \int_{-\infty}^{\infty} \mathrm{d}a_\omega\, \exp\left(-S[a;\bar{\Phi}]\right)$.

Let us assume that the φ_ω's are eigenfunctions of a certain differential operator, $\mathcal{L}$, which may depend on the background fields $\bar{\Phi}$, and which has properties similar to the negative Laplace-Beltrami operator, $-\bar{D}^2$. We suppose that $\mathcal{L}$ is built from covariant derivatives involving $\bar{g}_{\mu\nu}$ and the background Yang-Mills fields, if any, so that it is covariant under spacetime diffeomorphism and gauge-transformations. We assume an eigenvalue equation $\mathcal{L}\varphi_\omega = \Omega_\omega^2 \varphi_\omega$ with positive spectral values $\Omega_\omega^2 > 0$. The precise choice of $\mathcal{L}$ is arbitrary to a large extent. The only property of $\mathcal{L}$ we need is that it should associate small (large) distances on the rigid spacetime equipped with the metric $\bar{g}_{\mu\nu}$ to large (small) values of Ω_ω^2. A first (but for us not the essential) consequence is that we can now easily install a UV cutoff by restricting the ill-defined infinite product $\prod_\omega$ to only those ω's which satisfy $\Omega_\omega < \Omega_{\max}$. This implements a UV cutoff at the mass scale $\Omega_{\max}$.

More importantly for our purposes, we also introduce a smooth IR cutoff at a variable scale $k \leq \Omega_{\max}$ into the integral, replacing it with

$$Z_k = \prod_\omega{}' \int_{-\infty}^{\infty} \mathrm{d}a_\omega\, e^{-S[a;\bar{\Phi}]} e^{-\Delta S_k} \tag{1}$$

where the prime indicates the presence of the UV cutoff, and

$$\Delta S_k \equiv \frac{1}{2} \sum_\omega R_k(\Omega_\omega^2)\, a_\omega^2 \tag{2}$$

implements the IR cutoff. The extra piece in the bare action, ΔS_k, is designed in such a way that those φ_ω-modes which have eigenvalues $\Omega_\omega^2 \ll k^2$ get suppressed by a small factor $e^{-\Delta S_k} \ll 1$ in Eq. (1), while $e^{-\Delta S_k} = 1$ for the others. The function R_k is essentially arbitrary, except for its interpolating behavior between $R_k(\Omega_\omega^2) \sim k^2$ if $\Omega_\omega \ll k$ and $R_k(\Omega_\omega^2) = 0$ if $\Omega_\omega \gg k$.

The operator $\mathcal{L}$ defines the precise notion of 'coarse graining' field configurations. We regard the φ_ω's with $\Omega_\omega > k$ as the 'short wavelength' modes, to be integrated out first, and those with small eigenvalues $\Omega_\omega < k$ as the 'long wavelength' ones whose impact on the fluctuation's dynamics is not yet taken into account. This amounts to a diffeomorphism and gauge covariant generalization of the standard Wilsonian renormalization group, based on standard Fourier analysis on $\mathbb{R}^d$, to situations with arbitrary background fields $\bar{\Phi} = (\bar{g}_{\mu\nu}, \bar{A}_\mu, \cdots)$.

While helpful for the interpretation, it is often unnecessary to perform the expansion of $\hat{\varphi}(x)$ in terms of the $\mathcal{L}$-eigenfunctions explicitly. Rather, one thinks of (1) as a 'basis independent' functional integral

$$Z_k = \int \mathcal{D}'\hat{\varphi}\, e^{-S[\hat{\varphi};\bar{\Phi}]} e^{-\Delta S_k[\hat{\varphi};\bar{\Phi}]} \tag{3}$$

for which the eigen-basis of $\mathcal{L}$ plays no special role, while the operator $\mathcal{L}$ as such does so, of course. In particular the cutoff action ΔS_k is now rewritten with Ω_ω^2 replaced by $\mathcal{L}$ in the argument of R_k:

$$\Delta S_k[\hat{\varphi};\bar{\Phi}] = \frac{1}{2}\int \mathrm{d}^d x \sqrt{\bar{g}}\, \hat{\varphi}(x)\, R_k(\mathcal{L})\, \hat{\varphi}(x) \tag{4}$$

Note that at least when $k > 0$ the modified partition function Z_k depends on the respective choices for $\mathcal{L}$ and $\bar{\Phi}$ separately.

The family of k-dependent partition functions Z_k enjoys a simple property which is strikingly reminiscent of the C-theorem in 2 dimensions. Let us assume for simplicity that all component fields constituting $\hat{\varphi}$ are commuting, and that $\bar{\Phi}$ has been chosen k-independent. Then (3) is a (regularized, and convergent for appropriate S) purely bosonic integral with a positive integrand which, thanks to the suppression factor $e^{-\Delta S_k}$, decreases with increasing k. Therefore, Z_k and the 'entropy' $\ln Z_k$, are monotonically decreasing functions of the scale:

$$\partial_k \ln Z_k < 0 \tag{5}$$

The interpretation of (5) is clear: Proceeding from the UV to the IR by lowering the infrared cutoff scale, an increasing number of field modes get un-suppressed, thus contribute to the functional integral, and as a consequence the value of the partition function increases. Thus, in a sense, $\ln Z_k$ 'counts' the number of field modes that have been integrated out already. Before we can make this intuitive argument more precise we must introduce a number of technical tools at this point.

Running actions Introducing a source term for the fluctuation fields turns the partition functions $Z_k[J;\bar{\Phi}] \equiv e^{W_k[J;\bar{\Phi}]}$ into a generating functional:

$$e^{W_k[J;\bar{\Phi}]} = \int \mathcal{D}'\hat{\varphi}\, \exp\left(-S[\hat{\varphi};\bar{\Phi}] - \Delta S_k[\hat{\varphi};\bar{\Phi}] + \int \mathrm{d}^d x \sqrt{\bar{g}}\, J(x)\hat{\varphi}(x)\right) \tag{6}$$

Hence the $\bar{\Phi}$- and k-dependent expectation value $\langle\hat{\varphi}\rangle \equiv \varphi$ reads

$$\varphi(x) \equiv \langle\hat{\varphi}(x)\rangle = \frac{1}{\sqrt{\bar{g}(x)}} \frac{\delta W_k[J;\bar{\Phi}]}{\delta J(x)} \tag{7}$$

If we can solve this relation for J as a functional of $\bar{\Phi}$, the definition of the Effective Average Action (EAA), essentially the Legendre transform of W_k, may be written as

$$\Gamma_k[\varphi;\bar{\Phi}] = \int \mathrm{d}^d x \sqrt{\bar{g}}\, \varphi(x) J(x) - W_k[J;\bar{\Phi}] - \Delta S_k[\varphi;\bar{\Phi}] \tag{8}$$

with the solution to (7) inserted, $J \equiv J_k[\varphi;\bar{\Phi}]$. In the general case, Γ_k is the Legendre-Fenchel transform of W_k, with ΔS_k subtracted.

The EAA gives rise to a source-field relationship which includes an explicit cutoff term linear in the fluctuation field:

$$\frac{1}{\sqrt{\bar{g}}} \frac{\delta \Gamma_k[\varphi;\bar{\Phi}]}{\delta \varphi(x)} + \mathcal{R}_k[\bar{\Phi}]\varphi(x) = J(x) \tag{9}$$

Here and in the following we write $\mathcal{R}_k \equiv R_k(\mathcal{L})$, and the notation $\mathcal{R}_k[\bar{\Phi}]$ is used occasionally to emphasize that the cutoff operator may depend on the background fields. The solution to (9), and more generally all fluctuation correlators $\langle\hat{\varphi}(x_1)\cdots\hat{\varphi}(x_n)\rangle$ obtained by multiple differentiation of Γ_k, are functionally dependent on the background, e.g. $\varphi(x) \equiv \varphi_k[J;\bar{\Phi}](x)$. For the expectation value of the full, i.e. un-decomposed field $\hat{\Phi} = \bar{\Phi} + \hat{\varphi}$ we employ the notation $\Phi = \bar{\Phi} + \varphi$ with $\Phi \equiv \langle\hat{\Phi}\rangle$ and $\varphi \equiv \langle\hat{\varphi}\rangle$. Using the complete field Φ instead of φ as the second independent variable, accompanying $\bar{\Phi}$, entails the 'bi-field' variant of the EAA,

$$\Gamma_k[\Phi,\bar{\Phi}] \equiv \Gamma_k[\varphi;\bar{\Phi}]\big|_{\varphi=\Phi-\bar{\Phi}} \tag{10}$$

which, in particular, is always 'bi-metric': $\Gamma_k[g_{\mu\nu},\cdots,\bar{g}_{\mu\nu},\cdots]$.

Organizing the terms contributing to $\Gamma_k[\varphi;\bar{\Phi}]$ according to their *level*, i.e. their degree of homogeneity in the φ's, we assume that the EAA admits a *level expansion* of the form $\Gamma_k[\varphi;\bar{\Phi}] = \sum_{p=0}^{\infty} \check{\Gamma}_k^p[\varphi;\bar{\Phi}]$ where $\check{\Gamma}_k^p[c\,\varphi;\bar{\Phi}] = c^p\, \check{\Gamma}_k^p[\varphi;\bar{\Phi}]$ for any $c > 0$.

Self-consistent backgrounds We are interested in how the dynamics of the fluctuations $\hat{\varphi}$ depends on the environment they are placed in, the background metric $\bar{g}_{\mu\nu}$, for instance, and the other classical fields collected in $\bar{\Phi}$. It would be instructive to know if there exist special backgrounds in which the fluctuations are particularly 'tame' such that, for vanishing external source, they consists in at most small oscillations about a stable equilibrium, with a vanishing mean: $\varphi \equiv \langle\hat{\varphi}\rangle = 0$. Such distinguished backgrounds $\bar{\Phi} \equiv \bar{\Phi}^{\mathrm{sc}}$ are referred to as *self-consistent* (sc) since, if we prepare the system in one of those, the expectation value of the field

$\langle\hat{\Phi}\rangle = \Phi = \bar{\Phi}$ does not get changed by violent $\hat{\varphi}$-excitations that, generically, can shift the point of equilibrium. From Eq. (9) we obtain the following condition $\bar{\Phi}^{\rm sc}$ must satisfy (since $J = 0$ here by definition):

$$\frac{\delta}{\delta\varphi(x)}\Gamma_k[\varphi;\bar{\Phi}]\big|_{\varphi=0,\bar{\Phi}=\bar{\Phi}_k^{\rm sc}} = 0 \tag{11}$$

This is the *tadpole equation* from which we can compute the self-consistent background configurations, if any. In general $\bar{\Phi}^{\rm sc} \equiv \bar{\Phi}_k^{\rm sc}$ will have an explicit dependence on k. A technically convenient feature of (11) is that it no longer contains the somewhat disturbing $\mathcal{R}_k\varphi$-term that was present in the general field Eq. (9). Self-consistent backgrounds are equivalently characterized by Eq. (7),

$$\frac{\delta}{\delta J(x)}W_k[J;\bar{\Phi}]\big|_{J=0,\bar{\Phi}=\bar{\Phi}_k^{\rm sc}} = 0 \tag{12}$$

which again expresses the vanishing of the fluctuation's one-point function. Note that provided the level expansion exists we may replace (11) with

$$\frac{\delta}{\delta\varphi(x)}\check{\Gamma}_k^1[\varphi;\bar{\Phi}]\big|_{\varphi=0,\bar{\Phi}=\bar{\Phi}_k^{\rm sc}} = 0 \tag{13}$$

which involves only the level-(1) functional $\check{\Gamma}_k^1$. Later on in the applications this trivial observation has the important consequence that *self-consistent background field configurations* $\bar{\Phi}_k^{sc}(x)$ *can contain only running coupling constants of level* $p = 1$, that is, the couplings parameterizing the functional $\check{\Gamma}_k^1$ which is linear in φ.

In our later discussions the value of the EAA at $\varphi = 0$ will be of special interest. While it is still a rather complicated functional for a generic background where $\Gamma_k[0;\bar{\Phi}] = -W_k[J_k[0;\bar{\Phi}];\bar{\Phi}]$, the source which is necessary to achieve $\varphi = 0$ for self-consistent backgrounds is precisely $J = 0$, implying

$$\Gamma_k[0;\bar{\Phi}_k^{\rm sc}] \equiv \check{\Gamma}_k^0[0;\bar{\Phi}_k^{\rm sc}] = -W_k[0;\bar{\Phi}_k^{\rm sc}] \tag{14}$$

Here we also indicated that in a level expansion only the $p = 0$ term of Γ_k survives putting $\varphi = 0$. Note that $\Gamma_k[0;\bar{\Phi}_k^{\rm sc}]$ can contain only couplings of the levels $p = 0$ and $p = 1$, respectively, the former entering via $\check{\Gamma}_k^0$, the latter via $\bar{\Phi}_k^{\rm sc}$.

FIDE, FRGE, and WISS The EAA satisfies a number of important exact functional equations which include a functional integro-differential equation (FIDE), the functional RG equation (FRGE), the Ward identity for the Split-Symmetry (WISS), and the BRS-Ward identity.

In full generality, the FIDE reads

$$e^{-\Gamma_k[\varphi;\bar{\Phi}]} = \int \mathcal{D}'\hat{\varphi}\,\exp\left(-S[\hat{\varphi};\bar{\Phi}] - \Delta S_k[\hat{\varphi};\bar{\Phi}] + \int \mathrm{d}^d x\,\hat{\varphi}(x)\frac{\delta\Gamma_k}{\delta\varphi(x)}[\varphi;\bar{\Phi}]\right)$$

The last term on its RHS, the one linear in $\hat{\varphi}$, vanishes if the background is self-consistent and, in addition, $\varphi = 0$ is inserted:

$$\exp\left(-\Gamma_k[0;\bar{\Phi}_k^{\rm sc}]\right) = \int \mathcal{D}'\hat{\varphi}\, \exp\left(-S[\hat{\varphi};\bar{\Phi}_k^{\rm sc}] - \Delta S_k[\hat{\varphi};\bar{\Phi}_k^{\rm sc}]\right) \tag{15}$$

We shall come back to this important identity soon.

Another exact relation satisfied by the EAA is the FRGE,

$$k\partial_k\Gamma_k[\varphi;\bar{\Phi}] = \frac{1}{2}{\rm STr}\left[\left(\Gamma_k^{(2)}[\varphi;\bar{\Phi}] + \mathcal{R}_k[\bar{\Phi}]\right)^{-1} k\partial_k\mathcal{R}_k[\bar{\Phi}]\right] \tag{16}$$

comprising the Hessian matrix of the fluctuation derivatives $\Gamma_k^{(2)} \equiv \delta^2\Gamma_k/\delta\varphi^2$. The supertrace 'STr' in (16) provides the additional minus sign which is necessary for the φ-components with odd Grassmann parity, Faddeev-Popov ghosts and fermions.

The action $\Gamma_k[\Phi,\bar{\Phi}]$ satisfies the following exact functional equation which governs the 'extra' background dependence which it has over and above the one which combines with the fluctuations to form the full field $\Phi \equiv \bar{\Phi} + \varphi$:

$$\frac{\delta}{\delta\bar{\Phi}(x)}\Gamma_k[\Phi,\bar{\Phi}] = \frac{1}{2}{\rm STr}\left[\left(\Gamma_k^{(2)}[\Phi,\bar{\Phi}] + \mathcal{R}_k[\bar{\Phi}]\right)^{-1} \frac{\delta}{\delta\bar{\Phi}(x)}S_{\rm tot}^{(2)}[\Phi,\bar{\Phi}]\right] \tag{17}$$

Here $S_{\rm tot}^{(2)}$ is the Hessian of $S_{\rm tot} = S + \Delta S_k$ with respect to Φ, where S includes gauge fixing and ghost terms. Equation (17) is the Ward identity induced by the split-symmetry transformations $\delta\varphi = \varepsilon$, $\delta\bar{\Phi} = -\varepsilon$, hence the abbreviation 'WISS'. First obtained in [22] for Yang-Mills theory, extensive use has been made of (17) in quantum gravity [23] as a tool to assess the degree of split-symmetry breaking and the reliability of certain truncations [24].

Pointwise monotonicity From the definition of the EAA by a Legendre transform it follows that, for all $\bar{\Phi}$, the sum $\Gamma_k + \Delta S_k$ is a convex functional of φ, and that $\Gamma_k^{(2)} + \mathcal{R}_k$ is a strictly positive definite operator which can be inverted at all scales $k \in (0,\infty)$. Now let us suppose that the theory under consideration contains Grassmann-even fields only. Then the supertrace in (16) amounts to the ordinary, and convergent trace of a positive operator so that the FRGE implies

$$k\partial_k\Gamma_k[\varphi;\bar{\Phi}] \geq 0 \quad \text{at all fixed } \varphi,\ \bar{\Phi}. \tag{18}$$

Thus, at least in this class of distinguished theories the EAA, evaluated at any fixed pair of arguments φ and $\bar{\Phi}$, is a monotonically increasing function of k. With other words, *lowering k from the UV towards the IR the value of $\Gamma_k[\varphi;\bar{\Phi}]$ decreases monotonically*. We refer to this property as *pointwise monotonicity* in order to emphasize that it applies at all points of field space, $(\varphi,\bar{\Phi})$, separately.

In presence of fields with odd Grassmann parity, fermions and Faddeev-Popov ghosts, the RHS of the FRGE is no longer obviously non-negative. However, if the

only Grassmann-odd fields are ghosts the pointwise monotonicity (18) can still be made a general property of the EAA, the reason being as follows. At least when one implements the gauge fixing condition strictly, it cuts-out a certain subspace of the space of fields $\hat{\Phi}$ to be integrated over, namely the gauge orbit space. Hereby the integral over the ghosts represents the measure on this subspace, the Faddeev-Popov determinant. The subspace and its geometrical structures are invariant under the RG flow, however. Hence the EAA pertaining to the manifestly Grassmann-even integral *over the subspace* is of the kind considered above, and the argument implying (18) should therefore be valid again. For a more detailed form of this argument we must refer to [28]. From now on we shall make the explicit assumption, however, that the sets Φ and $\bar{\Phi}$ do not contain fermions.

Monotonicity vs. stationarity The EAA evaluated at fixed arguments shares the monotonicity property with a C-function. However, $\Gamma_k[\varphi;\bar{\Phi}]$ is not stationary at fixed points. In order to see why, and how to improve the situation, some care is needed concerning the interplay of dimensionful and dimensionless variables, to which we turn next.

(A) Let us assume that the space constituted by the functionals of φ and $\bar{\Phi}$ admits a basis $\{I_\alpha\}$ so that we can expand the EAA as

$$\Gamma_k[\varphi;\bar{\Phi}] = \sum_\alpha \bar{u}_\alpha(k)\, I_\alpha[\varphi;\bar{\Phi}] \tag{19}$$

with dimensionful running coupling constants $\bar{u} \equiv (\bar{u}_\alpha)$. They obey a FRGE in component form, $k\partial_k \bar{u}_\alpha(k) = \bar{b}_\alpha(\bar{u}(k);k)$, whereby the functions $\bar{b}_\alpha$ are defined by the expansion $\mathrm{Tr}[\cdots] = \sum_\alpha \bar{b}_\alpha(\bar{u}(k);k)\, I_\alpha[\varphi;\bar{\Phi}]$.

(B) Denoting the canonical mass dimension[1] of the running couplings by $[\bar{u}_\alpha] \equiv d_\alpha$, their dimensionless counterparts are defined by $u_\alpha \equiv k^{-d_\alpha}\bar{u}_\alpha$. In terms of the dimensionless couplings the expansion of Γ_k reads

$$\Gamma_k[\varphi;\bar{\Phi}] = \sum_\alpha u_\alpha(k) k^{d_\alpha} I_\alpha[\varphi;\bar{\Phi}] \tag{20}$$

Now observe that since Γ_k is dimensionless the basis elements have dimensions $\big[I_\alpha[\varphi;\bar{\Phi}]\big] = -d_\alpha$. Purely by dimensional analysis, this implies that[2]

$$I_\alpha[c^{[\varphi]}\varphi; c^{[\bar{\Phi}]}\bar{\Phi}] = c^{-d_\alpha} I_\alpha[\varphi;\bar{\Phi}] \quad \text{for any constant } c>0. \tag{21}$$

[1] Our conventions are as follows. We use dimensionless coordinates, $[x^\mu] = 0$. Then $[\mathrm{d}s^2] = -2$ implies that all components of the various metrics have $[\hat{g}_{\mu\nu}] = [\bar{g}_{\mu\nu}] = [g_{\mu\nu}] = -2$, and likewise for the fluctuations: $[\hat{h}_{\mu\nu}] = [h_{\mu\nu}] = -2$.

[2] We use the notation $c^{[\varphi]}\varphi \equiv \{c^{[\varphi_i]}\varphi_i\}$ for the set in which each field is rescaled according to its individual canonical dimension.

This relation expresses the fact that the nontrivial dimension of I_α is entirely due to that of its field arguments; there are simply no other dimensionful quantities available after the k-dependence has been separated off. Using (21) for $c = k^{-1}$ yields the dimensionless monomials

$$k^{d_\alpha} I_\alpha[\varphi; \bar{\Phi}] = I_\alpha[k^{-[\varphi]}\varphi; k^{-[\bar{\Phi}]}\bar{\Phi}] \equiv I_\alpha[\tilde{\varphi}; \tilde{\bar{\Phi}}] \tag{22}$$

Here we introduced the sets of dimensionless fields,

$$\tilde{\varphi}(x) \equiv k^{-[\varphi]}\varphi(x), \qquad \tilde{\bar{\Phi}}(x) \equiv k^{-[\bar{\Phi}]}\bar{\Phi}(x) \tag{23}$$

which include, for instance, the dimensionless metric and its fluctuations:

$$\tilde{h}_{\mu\nu}(x) \equiv k^2 h_{\mu\nu}(x), \qquad \tilde{\bar{g}}_{\mu\nu}(x) \equiv k^2 \bar{g}_{\mu\nu}(x) \tag{24}$$

Exploiting (22) in (20) we obtain the following representation of the EAA which is entirely in terms of dimensionless quantities[3] now:

$$\Gamma_k[\varphi; \bar{\Phi}] = \sum_\alpha u_\alpha(k)\, I_\alpha[\tilde{\varphi}; \tilde{\bar{\Phi}}] \;\equiv\; \mathcal{A}_k[\tilde{\varphi}; \tilde{\bar{\Phi}}] \tag{25}$$

Alternatively, one might wish to make its k-dependence explicit, writing,

$$\Gamma_k[\varphi; \bar{\Phi}] = \sum_\alpha u_\alpha(k)\, I_\alpha[k^{-[\varphi]}\varphi; k^{-[\bar{\Phi}]}\bar{\Phi}] \tag{26}$$

In the second equality of (25) we introduced the new functional $\mathcal{A}_k$ which, by definition, is numerically equal to Γ_k, but its natural arguments are the dimensionless fields $\tilde{\varphi}$ and $\tilde{\bar{\Phi}}$. Hence the k-derivative of $\mathcal{A}_k[\tilde{\varphi}, \tilde{\bar{\Phi}}]$ is to be performed at fixed $(\tilde{\varphi}, \tilde{\bar{\Phi}})$, while the analogous derivative of $\Gamma_k[\varphi; \bar{\Phi}]$ refers to fixed dimensionful arguments:

$$k\partial_k \mathcal{A}_k[\tilde{\varphi}; \tilde{\bar{\Phi}}] = \sum_\alpha k\partial_k u_\alpha(k)\, I_\alpha[\tilde{\varphi}; \tilde{\bar{\Phi}}] \tag{27a}$$

$$k\partial_k \Gamma_k[\varphi; \bar{\Phi}] = \sum_\alpha \left\{k\partial_k u_\alpha(k) + d_\alpha u_\alpha(k)\right\} k^{d_\alpha}\, I_\alpha[\varphi; \bar{\Phi}] \tag{27b}$$

(C) The *dimensionless* couplings $u \equiv (u_\alpha)$ can serve as local coordinates on *theory space*, $\mathcal{T}$. By definition, the 'points' of $\mathcal{T}$ are functionals $\mathcal{A}$ depending on dimensionless arguments: $\mathcal{A}[\tilde{\varphi}; \tilde{\bar{\Phi}}] = \sum_\alpha u_\alpha\, I_\alpha[\tilde{\varphi}; \tilde{\bar{\Phi}}]$. Geometrically speaking,

[3] Here one should also switch from k to the manifestly dimensionless 'RG time' $t \equiv \ln(k) + \text{const}$, but we shall not indicate this notationally.

RG trajectories are curves $k \mapsto \mathcal{A}_k = \sum_\alpha u_\alpha(k)\, I_\alpha \in \mathcal{T}$ that are everywhere tangent to

$$k\partial_k \mathcal{A}_k = \sum_\alpha \beta_\alpha(u(k))\, I_\alpha \tag{28}$$

The functions β_α, components of a vector field $\boldsymbol{\beta}$ on $\mathcal{T}$, are obtained by translating $k\partial_k \bar{u}_\alpha(k) = \bar{b}_\alpha(\bar{u}(k); k)$ into the dimensionless language. This leads to the autonomous system of differential equations

$$k\partial_k u_\alpha(k) \equiv \beta_\alpha(u(k)) = -d_\alpha u_\alpha(k) + b_\alpha(u(k)) \tag{29}$$

Here b_α, contrary to its dimensionful precursor $\bar{b}_\alpha$, has no explicit k-dependence, thus defining an RG-time independent vector field, the 'RG flow' $(\mathcal{T}, \boldsymbol{\beta})$.

If the flow has a fixed point at some u^*, i.e. $\beta_\alpha(u^*) = 0$, the 'velocity' of any trajectory passing this point vanishes there, $k\partial_k u_\alpha = 0$. Hence by (28) the action $\mathcal{A}_k$ becomes stationary there, that is, its scale derivative vanishes pointwise,

$$k\partial_k \mathcal{A}_k[\tilde{\varphi}; \tilde{\bar{\Phi}}] = 0 \qquad \text{for all fixed } \tilde{\varphi},\ \tilde{\bar{\Phi}}\,. \tag{30}$$

So the entire functional $\mathcal{A}_k$ approaches a limit, $\mathcal{A}_* = \sum_\alpha u^*_\alpha I_\alpha$. The standard EAA instead keeps running even in the fixed point regime:

$$\Gamma_k[\varphi; \bar{\Phi}] = \sum_\alpha u^*_\alpha\, k^{d_\alpha}\, I_\alpha[\varphi; \bar{\Phi}] \quad \text{when} \quad u_\alpha(k) = u^*_\alpha\,. \tag{31}$$

(D) This brings us back to the 'defect' of Γ_k we wanted to repair: While $\Gamma_k[\varphi; \bar{\Phi}]$ was explicitly seen to decrease monotonically along RG trajectories, it does not come to a halt at fixed points in general. The redefined functional $\mathcal{A}_k$, instead, approaches a finite limit $\mathcal{A}_*$ at fixed points, but is it monotone along trajectories?

Unfortunately this is not the case, and the culprit is quite obvious, namely the $d_\alpha u_\alpha$-terms present in the scale derivative of Γ_k, but absent for $\mathcal{A}_k$. The positivity of the RHS of Eq. (27b) does not imply the positivity of the RHS of Eq. (27a), and *there is no obvious structural reason for* $k\partial_k \mathcal{A}_k[\tilde{\varphi}; \tilde{\bar{\Phi}}] \geq 0$ *at fixed* $\tilde{\varphi}$, $\tilde{\bar{\Phi}}$. The best we can get is the following lower bound for the scale derivative: $k\partial_k \mathcal{A}_k[\tilde{\varphi}; \tilde{\bar{\Phi}}] \geq -\sum_\alpha d_\alpha u_\alpha(k)\, I_\alpha[\tilde{\varphi}; \tilde{\bar{\Phi}}]$.

The proposal The complementary virtues of $\mathcal{A}_k$ and Γ_k with respect to monotonicity along trajectories and stationarity at critical points suggest the following strategy for finding a C-type function with better properties: Rather than considering the functionals pointwise, i.e. with fixed configurations of either the dimensionless or

dimensionful fields inserted, one should evaluate them at *explicitly scale dependent arguments*: $\mathscr{C}_k \stackrel{?}{=} \Gamma_k[\varphi_k;\bar{\Phi}_k] \equiv \mathcal{A}_k[\tilde{\varphi}_k;\tilde{\bar{\Phi}}_k]$. The hope is that $\varphi_k \equiv k^{[\varphi]}\tilde{\varphi}_k$, and $\bar{\Phi}_k \equiv k^{[\bar{\Phi}]}\tilde{\bar{\Phi}}_k$ can be given a k-dependence which is intermediate between the two extreme cases $(\varphi, \bar{\Phi}) = \text{const}$ and $(\tilde{\varphi}, \tilde{\bar{\Phi}}) = \text{const}$, respectively, so as to preserve as much as possible of the monotonicity properties of Γ_k, while rendering $\mathscr{C}_k$ stationary at fixed points of the RG flow.

The most promising candidate which we could find so far is

$$\mathscr{C}_k = \Gamma_k[0;\bar{\Phi}_k^{\rm sc}] = \mathcal{A}_k[0;\tilde{\bar{\Phi}}_k^{\rm sc}] \tag{32}$$

Here the fluctuation argument is set to zero, $\varphi_k \equiv 0$, and for the background we choose a self-consistent one, $\bar{\Phi}_k^{\rm sc}$, a solution to the tadpole equation (11), or equivalently its dimensionless variant

$$\frac{\delta}{\delta\tilde{\varphi}(x)}\mathcal{A}_k[\tilde{\varphi};\tilde{\bar{\Phi}}]\big|_{\tilde{\varphi}=0,\,\tilde{\bar{\Phi}}=\tilde{\bar{\Phi}}_k^{\rm sc}} = 0 \tag{33}$$

The function $k \mapsto \mathscr{C}_k$ defined by Eq. (32) has a number of interesting properties to which we turn next.

(i) Stationarity at critical points. When the RG trajectory approaches a fixed point, $\mathcal{A}_k[\tilde{\varphi};\tilde{\bar{\Phi}}]$ approaches $\mathcal{A}_*[\tilde{\varphi};\tilde{\bar{\Phi}}]$ pointwise. Furthermore, the tadpole equation (33) becomes $(\delta\mathcal{A}_*/\delta\tilde{\varphi})[0;\tilde{\bar{\Phi}}_*] = 0$. It is k-independent, and so is its solution, $\tilde{\bar{\Phi}}_*$. Thus $\mathscr{C}_k$ approaches a well defined, finite constant:

$$\mathscr{C}_k \xrightarrow{\rm FP} \mathscr{C}_* = \mathcal{A}_*[0;\tilde{\bar{\Phi}}_*] \tag{34}$$

Of course we can write this number also as $\mathscr{C}_* = \Gamma_k[0;k^{[\bar{\Phi}]}\tilde{\bar{\Phi}}_*]$ wherein the explicit and the implicit scale dependence of the EAA cancel exactly when a fixed point is approached.

(ii) Stationarity at classicality. In a classical regime ('CR'), by definition, $\bar{b}_\alpha \to 0$, so that the *dimensionful* couplings stop running: $\bar{u}_\alpha(k) \to \bar{u}_\alpha^{\rm CR} = \text{const}$. Thus, by (19), Γ_k approaches $\Gamma_{\rm CR} = \sum_\alpha \bar{u}_\alpha^{\rm CR} I_\alpha$ pointwise. Hence the dimensionful version of the tadpole equation, (11), becomes k-independent, and the same is true for its solution, $\bar{\Phi}_{\rm CR}^{\rm sc}$. So, when the RG trajectory approaches a classical regime, $\mathscr{C}_k$ asymptotes a constant:

$$\mathscr{C}_k \xrightarrow{\rm CR} \mathscr{C}_{\rm CR} = \Gamma_{\rm CR}[0;\bar{\Phi}_{\rm CR}^{\rm sc}] \tag{35}$$

Alternatively we can write $\mathscr{C}_{\rm CR} = \mathcal{A}_k[0;k^{-[\bar{\Phi}]}\bar{\Phi}_{\rm CR}^{\rm sc}]$ where it is now the explicit and implicit k-dependence of $\mathcal{A}_k$ which cancel mutually.

We observe that there is a certain analogy between 'criticality' and 'classicality', in the sense that dimensionful and dimensionless couplings exchange

their roles. The difference is that the former situation is related to special *points* of theory space, while the latter concerns extended *regions* in $\mathcal{T}$. In those regions, $\mathcal{A}_k$ keeps moving as $\mathcal{A}_k[\cdot] = \sum_\alpha \bar{u}_\alpha^{\mathrm{CR}}\, k^{-d_\alpha}\, I_\alpha[\cdot]$. Nevertheless it is natural, and of particular interest in quantum gravity, to apply a (putative) C-function not only to crossover trajectories in the usual sense which connect two fixed points, but also to *generalized crossover transitions* where one of the fixed points is replaced by a classical regime.

(iii) Monotonicity at exact split-symmetry. If split-symmetry is exact in the sense that $\Gamma_k[\varphi;\bar{\Phi}]$ depends on the single independent field variable $\bar{\Phi}+\varphi \equiv \Phi$ only, and the theory is one of those for which pointwise monotonicity (18) holds true, then $k \mapsto \mathscr{C}_k$ is a monotonically increasing function of k. In fact, differentiating (32) and using the chain rule yields

$$\partial_k \mathscr{C}_k = (\partial_k \Gamma_k)\,[0;\bar{\Phi}_k^{\mathrm{sc}}] + \int \mathrm{d}^d x \left(\partial_k \bar{\Phi}_k^{\mathrm{sc}}(x)\right) \left(\frac{\delta \Gamma_k}{\delta \bar{\Phi}(x)} - \frac{\delta \Gamma_k}{\delta \varphi(x)} \right)\Bigg|_{\varphi=0,\,\bar{\Phi}=\bar{\Phi}_k^{\mathrm{sc}}} \tag{36}$$

In the first term on the RHS of (36) the derivative ∂_k hits only the explicit k-dependence of the EAA. By Eq. (18) we know that this contribution is non-negative. The last term, the $\delta/\delta\varphi$-derivative, is actually zero by the tadpole equation (11). Including it here it becomes manifest that the integral term in (36) vanishes when Γ_k depends on φ and $\bar{\Phi}$ only via the combination $\varphi+\bar{\Phi}$. Thus we have shown that

$$\partial_k \mathscr{C}_k \geq 0 \qquad \text{at exact split-symmetry} \tag{37}$$

This is already close to what one should prove in order to establish $\mathscr{C}_k$ as a 'C-function'. In particular in theories that require no breaking of split-symmetry the integral term in (36) is identically zero and we know that $\partial_k \mathscr{C}_k \geq 0$ holds true.

Whether or not $\partial_k \mathscr{C}_k$ is really non-negative for all k depends on the size of the split-symmetry breaking the EAA suffers from. To prove monotonicity of $\mathscr{C}_k$ one would have to show on a case-by-case basis that the second term on the RHS of (36) never can override the first one, known to be non-negative, so as to render their sum negative. In the next section we shall perform this analysis in a truncation of Quantum Einstein Gravity, but by working directly with the definition $\mathscr{C}_k = \Gamma_k[0;\bar{\Phi}_k^{\mathrm{sc}}]$ instead of Eq. (36).

Relating $\mathscr{C}_k$ to a spectral density Under special conditions, the EAA can be shown to literally 'count' field modes. For a sharp cutoff, and if $\mathcal{L} \equiv \Gamma_k^{(2)}[0;\bar{\Phi}_k^{\mathrm{sc}}]$ is such that it can be used as the cutoff operator, a formal calculation based upon the exact FRGE yields for the scale derivative of our candidate $\mathscr{C}$-function:

$$\frac{\mathrm{d}}{\mathrm{d}k^2}\mathscr{C}_k = \mathrm{Tr}\left[\delta\left(k^2 - \Gamma_k^{(2)}[0;\bar{\Phi}_k^{\mathrm{sc}}]\right)\right] \geq 0 \tag{38}$$

This is exactly the spectral density of the Hessian operator, for the sc-background and vanishing fluctuations, a manifestly non-decreasing function of k. If the k-dependence of $\Gamma_k^{(2)}$ is negligible relative to k^2, Eq. (38) is easily integrated:

$$\mathscr{C}_k = \mathrm{Tr}\left[\Theta\left(k^2 - \Gamma_k^{(2)}[0;\bar{\Phi}_k^{\mathrm{sc}}]\right)\right] + \mathrm{const} \tag{39}$$

Thus, at least under the special conditions described and when the spectrum is discrete, $\mathscr{C}_k$ indeed counts field modes in the literal sense of the word.

Regardless of the present approximation we define in general

$$\mathcal{N}_{k_1,k_2} \equiv \mathscr{C}_{k_2} - \mathscr{C}_{k_1} \tag{40}$$

Then, in the cases when the above assumptions apply and (39) is valid, $\mathcal{N}_{k_1,k_2}$ has a simple interpretation: it equals the number of eigenvalues between k_1^2 and $k_2^2 > k_1^2$ of the Hessian operator $\Gamma_k^{(2)}[0;\bar{\Phi}_k^{\mathrm{sc}}]$. When the assumptions leading to (39) are not satisfied, the interpretation of $\mathcal{N}_{k_1,k_2}$, and $\mathscr{C}_k$ in the first place, is less intuitive, but these quantities are well defined nevertheless.

3 Asymptotically Safe Quantum Gravity

Next, we test the above $\mathscr{C}_k$-candidate and apply it to Quantum Einstein Gravity, a theory which is asymptotically safe most probably, that is, all physically relevant RG trajectories start out in the UV, for k '$=$' ∞, at a point infinitesimally close to a non-Gaussian fixed point of the flow generated by the FRGE (16). When k is lowered, the trajectories run towards the IR, always staying within the fixed point's UV critical manifold, and ultimately approach the (dimensionless) ordinary effective action.

Dealing with pure metric gravity here we identify $\Phi \equiv (g_{\mu\nu}, \cdots)$, $\bar{\Phi} \equiv (\bar{g}_{\mu\nu}, \cdots)$, and $\varphi \equiv (h_{\mu\nu}, \cdots)$ as the dynamical, background, and fluctuation fields, respectively, where the dots stand for the entries due to the Faddeev-Popov ghosts. To make the analysis technically feasible we are going to truncate the corresponding theory space. Following Ref. [28] we focus here on the so-called bi-metric Einstein-Hilbert truncation. The corresponding ansatz for the EAA has the structure $\Gamma_k = \Gamma_k^{\mathrm{grav}}[g,\bar{g}] + \cdots$ where the dots represent gauge fixing and ghost terms which are taken to be k-independent and of classical form. The diffeomorphically invariant part of the action, Γ_k^{grav}, comprises two separate Einstein-Hilbert terms built from the dynamical metric, $g_{\mu\nu}$, and its background analog, $\bar{g}_{\mu\nu}$, respectively:

$$\begin{aligned}\Gamma_k^{\mathrm{grav}}[g,\bar{g}] = &-\frac{1}{16\pi G_k^{\mathrm{Dyn}}}\int \mathrm{d}^d x\sqrt{g}\left(R(g) - 2\Lambda_k^{\mathrm{Dyn}}\right)\\ &-\frac{1}{16\pi G_k^{\mathrm{B}}}\int \mathrm{d}^d x\sqrt{\bar{g}}\left(R(\bar{g}) - 2\Lambda_k^{\mathrm{B}}\right)\end{aligned} \tag{41}$$

The four couplings $\left(G_k^{\mathrm{Dyn}},\, \Lambda_k^{\mathrm{Dyn}},\, G_k^{\mathrm{B}},\, \Lambda_k^{\mathrm{B}}\right)$ represent k-dependent generalizations of the classical Newton and cosmological constant in the dynamical ('Dyn') and the background ('B') sector, respectively. In the simpler 'single-metric' variant of the Einstein-Hilbert truncation [13] the difference between $g_{\mu\nu}$ and $\bar{g}_{\mu\nu}$ is not resolved, and only one Einstein-Hilbert term is retained in Γ_k^{grav}. (Only in the gauge fixing term the two metrics appear independently.)

Expanding Eq. (41) in powers of the fluctuation field $h_{\mu\nu} = g_{\mu\nu} - \bar{g}_{\mu\nu}$ yields the level-expansion of the EAA:

$$\begin{aligned}\Gamma_k^{\mathrm{grav}}[h;\bar{g}] = &-\frac{1}{16\pi G_k^{(0)}}\int \mathrm{d}^d x\sqrt{\bar{g}}\left(R(\bar{g}) - 2\Lambda_k^{(0)}\right)\\ &-\frac{1}{16\pi G_k^{(1)}}\int \mathrm{d}^d x\sqrt{\bar{g}}\Big[-\bar{G}^{\mu\nu} - \Lambda_k^{(1)}\bar{g}^{\mu\nu}\Big]h_{\mu\nu} + \mathcal{O}(h^2)\end{aligned} \tag{42}$$

In the level-description, the background and dynamical couplings appear in certain combinations in front of invariants that have a definite level, i.e. order in $h_{\mu\nu}$. The two sets of coupling constants are related by $1/G_k^{(0)} = 1/G_k^{\mathrm{B}} + 1/G_k^{\mathrm{Dyn}}$ at level zero, and $G_k^{(p)} = G_k^{\mathrm{Dyn}}$ at all higher levels $p \geq 1$, and similarly for the Λ's. Thus, by hypothesis, all couplings of level $p \geq 1$ are assumed equal in this truncation. In either parametrization the truncated theory space is 4-dimensional.

The beta-functions describing the flow of the dimensionless couplings $g_k^I \equiv k^{d-2}G_k^I$ and $\lambda_k^I \equiv k^{-2}\Lambda_k^I$ for $I \in \{\mathrm{B}, \mathrm{Dyn}, (0), (1)\}$ were derived and analyzed in [13, 25, 29]. They were shown to give rise to both a trivial and a non-Gaussian fixed point (NGFP). A 2-dimensional projection of the RG flow onto the g^{Dyn}-λ^{Dyn}-plane is shown in Fig. 1. It is strikingly similar to the well known phase portrait of the corresponding single-metric truncation [16]. In this projection we can identify the same familiar classes of trajectories, namely those of type Ia, IIa, or IIIa, depending on whether the cosmological constant approaches $-\infty$, 0, or $+\infty$ in the IR. The type IIIa trajectories display a generalized crossover transition which connects a fixed point in the UV to a classical regime in the IR. The latter is located on the trajectory's lower, almost horizontal branch where $g,\, \lambda \ll 1$ [30].

Gravitational instantons For the bi-metric Einstein-Hilbert truncation, the tadpole equation boils down to

$$R_{\mu\nu}(\bar{g}_k^{\mathrm{sc}}) = \frac{2}{d-2}\Lambda_k^{(1)}\,\bar{g}_{k\,\mu\nu}^{\mathrm{sc}} \tag{43}$$

so that the self-consistent backgrounds are Einstein spaces, $\mathcal{M}$, with cosmological constant $\Lambda_k^{(1)}$. Furthermore, for $\mathscr{C}_k$ to be finite, the manifold $\mathcal{M}$ must have a finite volume. Trying to find backgrounds that exist for all scales the simplest situation arises when all metrics $\bar{g}_k^{\mathrm{sc}}$, $k \in [0, \infty)$ can be put on *the same smooth manifold* $\mathcal{M}$, leading in particular to the same spacetime topology at all scales, thus avoiding the delicate issue of a topological change. This situation is realized, for example, if

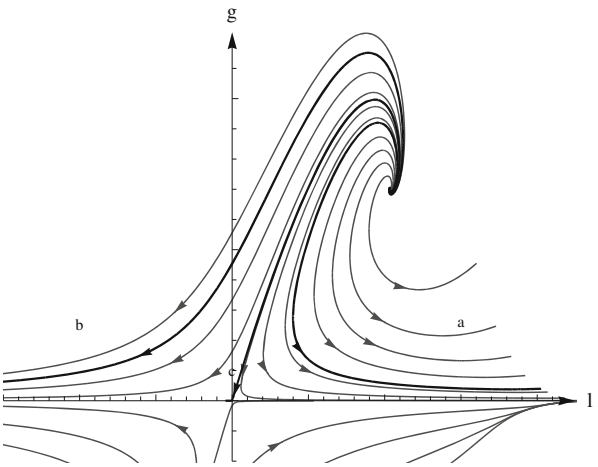


Fig. 1 Phase portrait on the g^{Dyn}-λ^{Dyn} plane as obtained by projecting the 4-dimensional bi-metric flow. This projection is qualitatively identical with the corresponding single-metric RG flow, displaying in particular the projection of a 4-dimensional non-Gaussian fixed point (NGFP)

the level-(1) cosmological constant is positive on all scales, as it is indeed the case along the type (IIIa) trajectories: $\Lambda_k^{(1)} > 0$, $k \in [0, \infty)$.

In the following we focus on this case, and we also specialize for $d = 4$. The requirement of a finite volume is then met by a well studied class of Einstein spaces which exist for an arbitrary positive value of the cosmological constant, namely certain 4-dimensional gravitational instantons, such as Euclidean de Sitter space, S^4, the Page metric, the product space $S^2 \times S^2$, or the Fubini-Study metric on the projective space $P_2(\mathbb{C})$ [31]. If $\mathring{g}_{\mu\nu}$ is one of these instanton metrics for some reference value of the cosmological constant, $\mathring{\Lambda}$, simple scaling arguments imply that $\bar{g}^{\mathrm{sc}}_{k\,\mu\nu} = \left(\mathring{\Lambda}/\Lambda_k^{(1)}\right) \mathring{g}_{\mu\nu}$ is a solution to the tadpole equation at any scale k. Inserting it into the truncation ansatz for Γ_k we find that the function $k \mapsto \mathscr{C}_k$ has the general structure

$$\mathscr{C}_k = \mathscr{C}(g_k^{(0)}, \lambda_k^{(0)}, \lambda_k^{(1)}) = \mathrm{Y}(g_k^{(0)}, \lambda_k^{(0)}, \lambda_k^{(1)})\, \mathcal{V}(\mathcal{M}, \mathring{g}) \tag{44}$$

Herein $\mathrm{Y}(\cdot) \equiv \mathscr{C}(\cdot)/\mathcal{V}$ is given by the following function over theory space:

$$\mathrm{Y}(g^{(0)}, \lambda^{(0)}, \lambda^{(1)}) = -\frac{2\lambda^{(1)} - \lambda^{(0)}}{g^{(0)}\,(\lambda^{(1)})^2} \qquad (d = 4) \tag{45}$$

Note that $\mathscr{C}$ depends on both the RG trajectory and on the specific solution to the running self-consistency condition that has been picked, along this very trajectory. In Eq. (44) those two dependencies factorize: the former enters via Y, the latter via

the dimensionless constant $\mathcal{V}(\mathcal{M}, \mathring{g}) \equiv \frac{1}{8\pi}\mathring{\Lambda}^2 \mathrm{Vol}(\mathcal{M}, \mathring{g})$. It characterizes the type of the gravitational instanton and can be shown to be actually independent of $\mathring{\Lambda}$. For S^4, for instance, its value is 3π, while the Fubini-Study metric has $\frac{9\pi}{2}$. The dependence on the trajectory, parametrized as $k \mapsto \left(g_k^{(0,1)}, \lambda_k^{(0,1)}\right)$, is obtained by evaluating a *scalar function on theory space* along this curve, namely $\mathrm{Y} : \mathcal{T} \to \mathbb{R}$, $\left(g^{(0,1)}, \lambda^{(0,1)}\right) \mapsto \mathrm{Y}(g^{(0)}, \lambda^{(0)}, \lambda^{(1)})$. It is defined at all points of $\mathcal{T}$ where $g^{(0)} \neq 0$ and $\lambda^{(1)} \neq 0$, and turns out to be actually independent of $g^{(1)}$.

We shall refer to $\mathrm{Y}_k \equiv \mathrm{Y}(g_k^{(0)}, \lambda_k^{(0)}, \lambda_k^{(1)}) \equiv \mathscr{C}_k/\mathcal{V}(\mathcal{M}, \mathring{g})$ and $\mathrm{Y}(\cdot) \equiv \mathscr{C}(\cdot)/\mathcal{V}(\mathcal{M}, \mathring{g})$ as the *reduced $\mathscr{C}_k$ and $\mathscr{C}(\cdot)$ functions,* respectively.

Numerical results In [25] the type IIIa trajectories on $\left(g^{(0)}, \lambda^{(0)}, g^{(1)}, \lambda^{(1)}\right)$-theory space were analyzed in detail. In [28] representative examples were computed numerically, and then $\mathscr{C}_k$ was evaluated along these trajectories. Concerning the monotonicity of $\mathscr{C}_k$, the results can be summarized as follows.

The set of RG trajectories that are asymptotically safe, i.e. originate in the UV at (or, more precisely, infinitesimally close to) the NGFP consists of two fundamentally different classes, namely those that are 'physical' and restore split-symmetry at their end point $k = 0$, and those which do not. (Within the present truncation, and according to the lowest order of the WISS, Eq. (17), intact split-symmetry amounts to $g_k^{(0)} = g_k^{(1)}$ and $\lambda_k^{(0)} = \lambda_k^{(1)}$.) *Along all trajectories that do restore split-symmetry, $\mathscr{C}_k$ was found to be perfectly monotone,* and stationary both at the NGFP and in the classical regime. Unphysical trajectories, not restoring split-symmetry in the IR, on the other hand, can give rise to a non-monotone behavior of $\mathscr{C}_k$.

A similar analysis was performed on the basis of the single-metric version of the Einstein-Hilbert truncation with a 2 dimensional theory space. It is less precise than its bi-metric counterpart as it hypothesizes perfect split-symmetry on all scales, something that can be true at best approximately because of the various unavoidable sources of symmetry breaking in the EAA (cutoff action ΔS_k, gauge fixing term). Regarding the monotonicity of $\mathscr{C}_k$, we found that *$\mathscr{C}_k$ fails to be monotone for any of the single-metric type IIIa trajectories.* The detailed analysis revealed that this failure is due to the (not quite unexpected) insufficiency of the single-metric approximation, rather than to a structural defect of the candidate $\mathscr{C}_k = \Gamma_k[0; \bar{\Phi}_k^{\mathrm{sc}}]$. For a typical RG trajectory, both the single- and bi-metric $\mathscr{C}_k$-functions are depicted in Fig. 2.

The numerical results [28] lend strong support to the following

Conjecture: *In the full theory, QEG in 4 dimensions, or in a sufficiently general truncation thereof, the proposed candidate for a 'C-like' function is a monotonically increasing function of k along all RG trajectories that restore split-symmetry in the IR and thus comply with the fundamental requirement of Background Independence.*

Crossover trajectories and entropy of de Sitter space The function $\mathscr{C}_k$ for truncated QEG is stationary at fixed points as well as in classical regimes. This is obvious from the following two alternative representations of the reduced

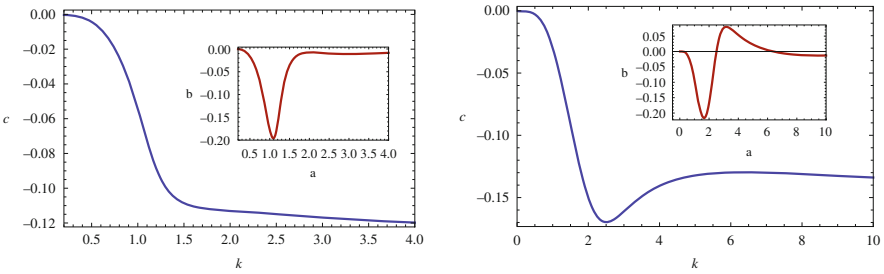


Fig. 2 The function $1/\mathrm{Y}_k$ computed from the bi-metric (*left diagram*) and the single-metric truncation (*right diagram*), respectively, along a representative type IIIa trajectory. The monotonicity of $\mathscr{C}_k$ is violated if the scale derivative of $1/\mathrm{Y}_k$, shown in the two insets, assumes positive values

$\mathscr{C}_k$-function:

$$\mathrm{Y}_k = -\frac{2\lambda_k^{(1)} - \lambda_k^{(0)}}{g_k^{(0)}\big(\lambda_k^{(1)}\big)^2} = -\frac{2\Lambda_k^{(1)} - \Lambda_k^{(0)}}{G_k^{(0)}\big(\Lambda_k^{(1)}\big)^2} \tag{46}$$

We see that Y_k, and hence $\mathscr{C}_k$ becomes stationary when the *dimensionless* couplings are at a fixed point of the flow, and also when the *dimensionful* ones become scale independent; this is the case in a classical regime ('CR') where, by definition, no physical RG effects occur. If Λ_{CR}^I and G_{CR}^I denote the constant values of the cosmological and Newton constants there, this regime amounts to the trivial canonical scaling $\lambda_k^I = k^{-2}\Lambda_{\mathrm{CR}}^I$ and $g_k^I = k^{d-2}G_{\mathrm{CR}}^I$.

As a result, there exists the possibility of generalized crossover transitions, not in the standard way from one fixed point to another, but rather from a fixed point to a classical regime or vice versa. Thereby $\mathscr{C}_k$ will always approach well defined stationary values $\mathscr{C}_*$ and $\mathscr{C}_{\mathrm{CR}}$ in the respective fixed point or classical regime. In quantum gravity, the investigations of such generalized crossover transitions is particularly important since one of its main tasks consists in explaining the emergence of a classical spacetime from the quantum regime.

Specializing again for an asymptotically safe type IIIa trajectory, the initial point in the UV is a non-Gaussian fixed point. For the limit $\mathscr{C}^{\mathrm{UV}} \equiv \lim_{k\to\infty}\mathscr{C}_k$ the bi-metric calculation yields $\mathscr{C}^{\mathrm{UV}} = \mathscr{C}_*$, with

$$\mathscr{C}_* = -\frac{2\lambda_*^{(1)} - \lambda_*^{(0)}}{g_*^{(0)}\big(\lambda_*^{(1)}\big)^2}\,\mathcal{V}(\mathcal{M}, \mathring{g}) \tag{47}$$

According to the Einstein-Hilbert results for the NGFP, $-\mathscr{C}_*/\mathcal{V}(\mathcal{M}, \mathring{g})$ is a positive number of order unity, presumably between about 4 and 8. Concerning the opposite limit $\mathscr{C}^{\mathrm{IR}} = \lim_{k\to 0}\mathscr{C}_k$, the trajectory describes a generalized crossover, enters a classical regime, and restores split-symmetry for $k \to 0$. This entails $\mathscr{C}^{\mathrm{IR}} = \mathscr{C}_{\mathrm{CR}}$

where

$$\mathscr{C}_{\mathrm{CR}} = -\frac{\mathcal{V}(\mathcal{M}, \mathring{g})}{G_{\mathrm{CR}}\Lambda_{\mathrm{CR}}} \tag{48}$$

Here we exploited that split-symmetry implies the values of G_{CR} and Λ_{CR} to be level independent.

We may conclude that *in an asymptotically safe theory of quantum gravity which is built upon a generalized crossover trajectory from criticality (the NGFP) to classicality the $\mathscr{C}_k$-function candidate implies the 'integrated $\mathscr{C}$-theorem' $\mathcal{N} \equiv \mathcal{N}_{0,\infty} = \mathscr{C}^{\mathrm{UV}} - \mathscr{C}^{\mathrm{IR}}$ with finite numbers $\mathscr{C}^{\mathrm{UV}}$, $\mathscr{C}^{\mathrm{IR}}$, and $\mathcal{N}$.*

This finiteness is in marked contrast to what standard perturbative field theory would predict. Clearly, the Asymptotic Safety of QEG is the essential prerequisite for this property since it is the non-Gaussian fixed point that assigns a well defined, computable value to $\mathscr{C}^{\mathrm{UV}}$.

The quantity $\mathcal{N}$ can be interpreted as a measure for the 'number of modes' which are integrated out while the cutoff is lowered from infinity to $k = 0$. The notion of 'counting' and the precise meaning of a 'number of field modes' is defined by the EAA itself, namely via the identification $\mathscr{C}_k = \Gamma_k[\bar{\Phi}_k^{\mathrm{sc}}, \bar{\Phi}_k^{\mathrm{sc}}]$. We saw in the previous section that, under special conditions, $\mathscr{C}_k$ is literally counting the $\Gamma_k^{(2)}$-eigenvalues in a given interval. However, generically we are dealing with a non-trivial generalization thereof which, strictly speaking, amounts to a *definition* of 'counting'. As such it is probably the most natural one from the perspective of the EAA and the geometry of theory space.

Let us consider a simple caricature of the real Universe, namely a family of de Sitter spaces along a type IIIa trajectory, whose classical regime in the IR has $\Lambda_{\mathrm{CR}} > 0$. Assuming it represents the real final state of the evolution, we have $\mathscr{C}^{\mathrm{IR}} = -3\pi/G_{\mathrm{CR}}\Lambda_{\mathrm{CR}} < 0$. Note that $|\mathscr{C}^{\mathrm{IR}}|$ equals precisely the well known semi-classical Bekenstein-Hawking entropy of de Sitter space.

If in particular $G_{\mathrm{CR}}\Lambda_{\mathrm{CR}} \ll 1$, corresponding to a very 'large' classical Universe, we have $|\mathscr{C}^{\mathrm{IR}}| \gg 1$, while $|\mathscr{C}^{\mathrm{UV}}| = \mathcal{O}(1)$ is invariably determined by the NGFP coordinates. As a consequence, the number $\mathcal{N}$ is completely dominated by the IR part of the trajectory:

$$\mathcal{N} = \mathscr{C}^{\mathrm{UV}} - \mathscr{C}^{\mathrm{IR}} \approx -\mathscr{C}^{\mathrm{IR}} \approx +\frac{3\pi}{G_{\mathrm{CR}}\Lambda_{\mathrm{CR}}} \gg 1 \tag{49}$$

Identifying Λ_{CR} and G_{CR} with the corresponding values measured in the real Universe we would find $\mathcal{N} \approx 10^{120}$.

Thus, in the sense explained above, the familiar Bekenstein-Hawking entropy of de Sitter space acquires a rather concrete interpretation, namely as the number of metric and ghost fluctuation modes that are integrated out between the NGFP in the UV and the classical regime in the IR. It plays a role analogous to the central charge of the IR conformal field theory in Zamolodchikov's case.

Beside monotonicity and stationarity, $\mathscr{C}_k$ has another essential property in common with a C-function: The limiting value $\mathscr{C}_*$ has a genuine inherent interpretation at the fixed point itself. It is a number characteristic of the NGFP which does not depend on the direction it is approached, and in this role it is analogous to the central charge. The interpretation of $\mathscr{C}_*$ is best known for the single-metric approximation ($g^{(0)} \approx g^{(1)}$, $\lambda^{(0)} \approx \lambda^{(1)}$) where, apart from inessential constants, it is precisely the inverse of the dimensionless combination $g_*\lambda_* = G_{k\to\infty}\Lambda_{k\to\infty}$. Its physical interpretation is that of an 'intrinsic' measure for the size of the cosmological constant at the fixed point, namely the limit of *the running cosmological constant in units of the running Planck mass* ($G_k^{-1/2}$). In numerous single-metric studies the product $g_*\lambda_*$ has been investigated, and it was always found that $g_*\lambda_*$ *is a universal quantity*, i.e. it is independent of the cutoff scheme and the gauge fixing, within the accuracy permitted by the approximation. In fact, typically the universality properties of $g_*\lambda_*$ were even much better than those of the critical exponents. Completely analogous remarks apply to the bi-metric generalization.

Concerning the finiteness of $\mathcal{N}$, the situation changes fundamentally if we try to define the function $k \mapsto \mathscr{C}_k$ along trajectories of the type Ia, those heading for a negative cosmological constant $\lambda^{\rm Dyn}$ after leaving the NGFP regime, and of type IIa, the single trajectory which crosses over from the NGFP to the Gaussian fixed point. For all type Ia trajectories, $\mathscr{C}_k$ becomes singular at some nonzero scale $k_{\rm sing} > 0$ when they pass $\lambda^{\rm Dyn} = 0$. As Eq. (45) shows, $\mathrm{Y}(\cdot)$ and $\mathscr{C}(\cdot)$ have a pole there so that $\mathscr{C}_k$ diverges in the limit $k \searrow k_{\rm sing}$. The number $\mathcal{N}_{k_{\rm sing},\infty}$ is infinite then, even though not all modes are integrated out yet. There is a non-trivial RG evolution also between $k_{\rm sing}$ and $k = 0$. The tadpole equation has qualitatively different solutions for $k > k_{\rm sing}$, $k = k_{\rm sing}$, and $k < k_{\rm sing}$, namely spherical, flat, and hyperbolic spaces, respectively (S^d, R^d, and H^d, say). This topology change prevents us from smoothly continuing the mode count across the $\lambda^{\rm Dyn} = 0$ plane. This is the reason why we mostly focused on type IIIa trajectories here.

4 Summary

The effective average action is a variant of the standard effective action which has an IR cutoff built in at a sliding scale k. At least for systems without fermions it possesses a natural mode counting and ('pointwise') monotonicity property which is strongly reminiscent of, but actually not equivalent to, Zamolodchikov's C-function in 2 dimensions. Motivated by this observation, and taking advantage of the structures and tools that are naturally provided by the manifestly non-perturbative EAA framework, we tried to find a map from the functional $\Gamma_k[\Phi, \bar{\Phi}]$ to a single real valued function $\mathscr{C}_k$ that shares two main properties with the C-function in 2 dimensions, namely monotonicity along RG trajectories and stationarity at RG fixed points. Such a map is unlikely to exist in full generality. In fact, an essential part of the research program we are proposing consists in finding suitable restrictions

on, or specializations of the *admissible trajectories* (restoring split-, or other symmetries, etc.), the *theory space* (with respect to field contents and symmetries), the underlying *space of fields* (boundary conditions, regularity requirements, etc.), and the *coarse graining methodology* (choice of cutoff, treatment of gauge modes, etc.) that will guarantee its existence. We motivated a specific candidate for a map of this kind, namely $\mathscr{C}_k = \Gamma_k[\bar{\Phi}_k^{\rm sc}, \bar{\Phi}_k^{\rm sc}]$ where $\bar{\Phi}_k^{\rm sc}$ is a running self-consistent background, a solution to the tadpole equation implied by Γ_k. This function $\mathscr{C}_k$ is stationary at fixed points, and a non-decreasing function of k provided the breaking of the split-symmetry which relates fluctuation fields and backgrounds is sufficiently weak. Thus, for a concrete system the task is to identify the precise conditions under which the split-symmetry violation does not destroy the monotonicity property of $\mathscr{C}_k$, and to give a corresponding proof then.

By means of a particularly relevant example, asymptotically safe QEG in 4 dimensions, we demonstrated that this strategy is viable in principle and can indeed lead to interesting candidates for 'C-like' functions under conditions which are not covered by the known c- and a-theorems. Within a sufficiently precise truncation of QEG, on a 4 dimensional theory space, we showed that $\mathscr{C}_k$ has exactly the desired properties of monotonicity and stationarity, provided it is based upon a physically meaningful RG trajectory, that is, one which leads to a restoration of Background-Independence once all field modes are integrated out.

Acknowledgements M. R. would like to thank the organizers of *Quantum Mathematical Physics* for their hospitality at Regensburg and for a particularly stimulating conference.

References

1. A.B. Zamolodchikov, Irreversibility of the flux of the renormalization group in a 2D field theory. JETP Lett. **43**, 730 (1986); Renormalization group and perturbation theory near fixed points in two-dimensional field theory. Sov. J. Nucl. Phys. **46**, 1090 (1987)
2. J.L. Cardy, Is there a c theorem in four-dimensions? Phys. Lett. B **215**, 749 (1988)
3. H. Osborn, Derivation of a four-dimensional c theorem. Phys. Lett. B **222**, 97 (1989); I. Jack, H. Osborn, Analogs for the c theorem for four-dimensional renormalizable field theories. Nucl. Phys. B **343**, 647 (1990)
4. A.H. Castro Neto, E. Fradkin, The thermodynamics of quantum systems and generalizations of Zamolodchikov's C theorem. Nucl. Phys. B **400**, 525 (1993)
5. I. Klebanov, S. Pufu, B. Safdi, F-theorem without supersymmetry. JHEP **1110**, 038 (2011)
6. A. Cappelli, D. Friedan, J.I. Latorre, C theorem and spectral representation. Nucl. Phys. B **352**, 616 (1991)
7. G.M. Shore, Phys. Lett. B **253** (1991); The C(F) theorem. Phys. Lett. B **256**, 407 (1991)
8. F. Bastianelli, Tests for c theorems in 4-D. Phys. Lett. B **369**, 249 (1996)
9. D. Anselmi, D.Z. Freedman, M.T. Grisaru, A.A. Johansen, Nonperturbative formulas for central functions of supersymmetric gauge theories. Nucl. Phys. B **526**, 543 (1998)
10. Z. Komargodski, A. Schwimmer, On renormalization group flows in four dimensions. JHEP **12**, 099 (2011)
11. M. Luty, J. Polchinski, R. Rattazi, The a-theorem and the asymptotics of 4D quantum field theory. JHEP **01**, 152 (2013)

12. S. Weinberg, in *General Relativity, an Einstein Centenary Survey*, ed. by S.W. Hawking, W. Israel (Cambridge University Press, Cambridge, 1979)
13. M. Reuter, Nonperturbative evolution equation for quantum gravity. Phys. Rev. D **57**, 971 (1998) and hep-th/9605030
14. O. Lauscher, M. Reuter, Ultraviolet fixed point and generalized flow equation of quantum gravity Phys. Rev. D **65**, 025013 (2002) and hep-th/0108040
15. O. Lauscher, M. Reuter, Flow equation of quantum Einstein gravity in a higher derivative truncation Phys. Rev. D **66**, 025026 (2002); Is quantum Einstein gravity nonperturbatively renormalizable? Class. Quantum Gravity **19**, 482 (2002) and hep-th/0110021
16. M. Reuter, F. Saueressig, Renormalization group flow of quantum gravity in the Einstein-Hilbert truncation. Phys. Rev. D **65**, 065016 (2002)
17. For a review on QEG and Asymptotic Safety and a comprehensive list of references see M. Reuter, F. Saueressig, Quantum Einstein gravity. New J. Phys. **14**, 055022 (2012)
18. M. Niedermaier, M. Reuter, The asymptotic safety scenario in quantum gravity. Living Rev. Relativ. **9**, 5 (2006); M. Reuter, F. Saueressig, in *Geometric and Topological Methods for Quantum Field Theory*, ed. by H. Ocampo, S. Paycha, A. Vargas (Cambridge University Press, Cambridge, 2010) arXiv:0708.1317; R. Percacci, in *Approaches to Quantum Gravity: Towards a New Understanding of Space, Time and Matter*, ed. by D. Oriti (Cambridge University Press, Cambridge, 2009) arXiv:0709.3851.
19. O. Lauscher, M. Reuter, in *Quantum Gravity,* ed. by B. Fauser, J. Tolksdorf, E. Zeidler (Birkhäuser, Basel, 2007)
20. M. Reuter, C. Wetterich, Average action for the Higgs model with Abelian gauge symmetry. Nucl. Phys. B **391**, 147 (1993); Running gauge coupling in three-dimensions and the electroweak phase transition. Nucl. Phys. B **408**, 91 (1993); C. Wetterich, Exact evolution equation for the effective potential. Phys. Lett. B **301**, 90 (1993); M. Reuter, C. Wetterich, Effective average action for gauge theories and exact evolution equations. Nucl. Phys. B **417**, 181 (1994); Exact evolution equation for scalar electrodynamics. Nucl. Phys. B **427**, 291 (1994)
21. A. Ashtekar, M. Reuter, C. Rovelli, *From General Relativity to Quantum Gravity* arXiv:1408.4336
22. M. Reuter, C. Wetterich, Gluon condensation in nonperturbative flow equations. Phys. Rev. D **56** 7893 (1997)
23. E. Manrique, M. Reuter, Bimetric truncations for quantum Einstein gravity and asymptotic safety. Ann. Phys. **325**, 785 (2010). arXiv:0907.2617
24. M. Reuter, H. Weyer, Conformal sector of quantum Einstein gravity in the local potential approximation: Non-Gaussian fixed point and a phase of unbroken diffeomorphism invariance Phys. Rev. D **80**, 025001 (2009) and arXiv:0804.1475
25. D. Becker, M. Reuter, En route to background independence: broken split-symmetry, and how to restore it with bi-metric average actions Ann. Phys. **350**, 225 (2014). arXiv:1404.4537
26. D. Becker, M. Reuter, Propagating gravitons vs. 'dark matter' in asymptotically safe quantum gravity. JHEP **1412**, 025 (2014). arXiv:1407.5848
27. E. Manrique, M. Reuter, Bare action and regularized functional integral of asymptotically safe quantum gravity. Phys. Rev. D **79**, 025008 (2009) and arXiv:0811.3888
28. D. Becker, M. Reuter, Towards a C-function in 4D quantum gravity. JHEP **1503**, 065 (2015) and arXiv:1412.0468
29. E. Manrique, M. Reuter, F. Saueressig, Bimetric renormalization group flows in quantum Einstein gravity. Ann. Phys. **326**, 463 (2011). arXiv:1006.0099
30. M. Reuter, H. Weyer, Quantum gravity at astrophysical distances? JCAP **0412** 001 (2004). hep-th/0410119
31. T. Eguchi, P. Gilkey, A. Hanson, Gravitation, Gauge theories and differential geometry. Phys. Rep. **66** 213 (1980) and references therein.

Systematic Renormalization at all Orders in the DiffRen and Improved Epstein–Glaser Schemes

José M. Gracia-Bondía

Contents

Abstract Proceeding by way of examples, we update the combinatorics of the treatment of Feynman diagrams with subdivergences in differential renormalization from more recent viewpoints in Epstein–Glaser renormalization in x-space.

Keywords Configuration space • Combinatorics of Feynman graphs • Epstein-Glaser renormalization • Differential renormalization.

Mathematics Subject Classification (2010). 46F10, 81T15, 81T18.

J.M. Gracia-Bondía (✉)
Department of Theoretical Physics, Universidad de Zaragoza, 50009 Zaragoza, Spain

BIFI Research Center, Universidad de Zaragoza, 50018 Zaragoza, Spain

Institute for Theoretical Physics, Universidad Autónoma, 28049 Madrid, Spain
e-mail: jmgb@unizar.es

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_3

1 Introduction

Ultraviolet divergent amplitudes of Feynman diagrams in x-space are given by functional expressions too singular at short distances to define distributions on all of space(-time). Quite often, however, they can be represented on their domain of definition as derivatives of *bona fide* distributions, and so extended to the whole space. "Differential renormalization" (DiffRen for short) in this sense does not need previous regularization steps. It was introduced by Freedman, Johnson and Latorre in a path-breaking article [1].

While that reference is a true *tour de force*, showing the calculational power of the method (and of its authors), it did not attempt to disentangle the combinatorics of successive renormalizations for non-primitive graphs in a systematic way. This task was taken up in later work in differential renormalization [2].

Differential renormalization remained popular during the nineties, to peter out in the third millennium. Now, a spate of papers [3–5] have recently dealt with renormalization in x-space in the spirit of the classic article by Epstein and Glaser [6], whose kinship with DiffRen is evident. Each of those solves the renormalization recursion in its own way. Among them, reference [4] adheres to DiffRen closely and improves it. Our aim here is to pedagogically revisit from its viewpoint the combinatorics of the "subtraction" of subdivergences in [2] as well, comparing methods and (hopefully) bringing improvement again.

As in the last-mentioned paper, for simplicity we deal mostly with the Euclidean massless ϕ_4^4 model.

2 The Importance of Degree

We start by a point of rigour, that some readers may wish to skip. Naturally the first step in [2] is to determine whether a given graph needs renormalization. The answer they give, in view of Weinberg's "power counting" theorem [7, 8], is to find the superficial degree of each generalized vertex (subgraph) in the graph. Now, that theorem yields a *sufficient* condition for renormalizability. While the question of improving on it is moot for scalar models, experience with renormalization of massless graphs suggests a less restrictive criterion. To wit, extension of log-homogeneous graphs in the sense of [3, 4] produces log-homogeneous graphs of the same order and higher degree. Whenever the extension can be made to a log-homogeneous graph of the *same* degree, we understand that we deal with a matter of (re)definition, the diagram is convergent, and no renormalization has taken place.

The subject is discussed in [3], but we deem it worthwhile to bring it here for completeness in our review of [2]. We show a truly trivial example in the Minkowski space M_4. The distribution $\delta(x^2)$ appears routinely in formulas for the propagators of free massless fields. However, its meaning is not altogether obvious. Given any distribution f on $\mathbb{R}$, one is able to define pullback distributions $f(P)$ on smooth hypersurfaces P (codimension 1 submanifolds) of M_4; in particular one defines $\delta(P)$.

However the lightcone $x^2 = 0$ is not smooth at the origin, where grad x^2 vanishes. Thus *prima facie* $\delta(x^2)$ is defined on $M_4 \setminus \{0\}$ only—as a homogeneous distribution of order -2. Consider, however, for small positive ε, the distributions:

$$\langle \delta_\pm(x^2 - \varepsilon), \phi \rangle = \int_\pm \phi \, \mu_\varepsilon,$$

where the integrals are respectively concentrated on the upper and lower sheet of the hyperboloid $\{ x : x^2 = \varepsilon \}$, and μ_ε is a Leray form such that $dx^2 \wedge \mu_\varepsilon = d^4x$. One can take $\mu_\varepsilon = \dfrac{d^3\boldsymbol{x}}{2t(r;\varepsilon)} := \dfrac{d^3\boldsymbol{x}}{2\sqrt{r^2+\varepsilon}}$ with $r \equiv |\boldsymbol{x}|$. Hence,

$$\langle \delta_\pm(x^2 - \varepsilon), \phi \rangle = \frac{1}{2} \int \frac{\phi(\pm\sqrt{r^2+\varepsilon}, \boldsymbol{x})}{\sqrt{r^2+\varepsilon}} \, d^3\boldsymbol{x} = 2\pi \int_0^\infty \frac{\bar{\phi}(\pm\sqrt{r^2+\varepsilon}, r)}{\sqrt{r^2+\varepsilon}} \, r^2 \, dr.$$

We have called $\bar{\phi}(t, r)$ the average value of ϕ on a sphere of radius r in $\boldsymbol{x}$-space. Then the limits as $\varepsilon \downarrow 0$,

$$\langle \delta_\pm(x^2), \phi \rangle = 2\pi \int_0^\infty \bar{\phi}(\pm r, r) \, r \, dr, \tag{1}$$

are obviously well defined, and they extend the previous $\delta(x^2)$.

The extension of $\delta(x^2)$ of course is not unique; but crucially the one just defined preserves Lorentz symmetry and keeps the *same* degree of homogeneity: we then reckon that no "renormalization" has taken place.[1]

A more sophisticated example is found in [3, Sect. 5]. The propagator of the free electromagnetic field is the quotient of a harmonic polynomial of degree 2 by the third power of x^2, and thus is logarithmically divergent by power counting. However, it does possess an homogeneous extension, therefore it is convergent in our more precise sense. The example offers little doubt, since, as is well known, it boils down to second derivatives of the massless propagator [9].

3 Dealing with a Three-Point Problem

Let us continue by pointing to another difference between DiffRen as practiced in [1, 2] and the (improved) Epstein–Glaser method [10]. In the former papers one finds an extension for the "fish" graph of the ϕ_4^4 model, with vertices $(0, x)$:

$$r_x[x^{-4}] = -\frac{1}{2} \, \Delta\left(x^{-2} \log \frac{|x|}{l} \right),$$

[1] The "original sin" still shows in that, whereas for $\varepsilon > 0$ we can indefinitely apply to $\delta_\pm(x^2 - \varepsilon)$ the usual derivation rules, the expression $\delta'(x^2)$ on M_4 is meaningless.

in the understanding that $l = 1/M$, where M is their mass scale; while, as explained in [4], we prefer

$$R_x[x^{-4}] = -\frac{1}{2}\left[\Delta\left(x^{-2}\log\frac{|x|}{l}\right) - \pi^2\,\delta(x)\right],$$

because $x^2 R_x[x^{-4}] = x^{-2}$, while $x^2 r_x[x^{-4}]$ fails to reproduce the convergent amplitude x^{-2}. The algebra property of [10] generalizes throughout into the "causal factorization property" of [3], which is the basis for a streamlined proof of the recursive renormalization of subdivergences.

Now, our lodestone to deal with recursive renormalization in [4] was a rule contained in the very illuminating paper [11]. It is written:

$$\langle R[\Gamma], \varphi\rangle = \langle R[\gamma], (\Gamma/\gamma)\,\varphi\rangle. \tag{2}$$

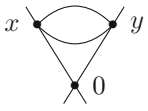
In this formula any subgraph γ of a given graph Γ is identified as a subset of the set of vertices of Γ and the set of *all* lines joining any two elements of this subset. There $R[\Gamma]$, $R[\gamma]$ and Γ/γ denote amplitudes, respectively for the renormalized graph and subgraph, and the bare cograph Γ/γ; the test function φ is supported outside the singular points of the latter. The rule works as a necessary and sufficient *prescription*: the $R[\gamma]$ are supposed known, and then $R[\Gamma]$ must conform to the formula above. It subsumes (the Euclidean version of) the causal factorization property, which allowed a streamlined proof of recursive renormalization in [3], but would be awkward in actual computation. Later we will show how rule (2) works when there are internal vertices in Γ, by means of an interesting six-loop diagram considered in [2].

In [2], on the other hand, it is claimed that recursive renormalization is effected by use of Bogoliubov's subtraction operators [12, Ch. 29]; another good reference for this method is [8]. For instance, according to them, the bare graph x^{-4}, with vertices $(x, 0)$, is renormalized by

$$r_{x,0}[x^{-4}] = (I - T_{x,0})x^{-4} \quad \text{with} \quad T_{x,0}\,x^{-4} := x^{-4} - \left(-\frac{1}{2}\,\Delta\left(x^{-2}\log\frac{|x|}{l}\right)\right).$$

Actually $T_{x,0}\,x^{-4}$ as written above makes no sense, since if we compare both its summands on the intersection of their natural domains we obtain zero. But it is obvious how to get rid notationally of this ugly contortion, which makes violence to DiffRen.

Let us start in earnest by considering, as the authors in that paper do, the example of the winecup graph or ice-cream ladder graph, devoid of internal vertices:



(In order to get closer to the notation in [2], we have exchanged vertices x and 0 in the formulae in [4].) We denote it  (x, y) for future use. The corresponding bare amplitude is given by

$$f(x,y) = \frac{1}{x^2 y^2 (x-y)^4}\,.$$

Both papers [1] and [4] consider a "partially renormalized" version of the winecup graph, for which the known formulas respectively yield:

$$r_{x,y}\big[x^{-2}y^{-2}(x-y)^{-4}\big] = -\frac{1}{2}\,x^{-2}y^{-2}\,\Delta\Big((x-y)^{-2}\log\frac{|x-y|}{l}\Big); \tag{3}$$

$$\begin{aligned} R_{x,y}\big[x^{-2}y^{-2}(x-y)^{-4}\big] &= -\frac{1}{2}\,x^{-2}y^{-2}\,\Delta\Big((x-y)^{-2}\log\frac{|x-y|}{l}\Big) \\ &\quad + \pi^2 x^{-4}\,\delta(x-y). \end{aligned}$$

The last expressions indeed make sense for all $(x, y) \neq (0, 0)$.

The first term on the right hand sides above is the one given in [2, Eq. 2.15]. Extension of the last term, not present there, to the thin diagonal (i.e., the whole graph), clearly is no problem. So we concentrate in extending the first: each of the factors in $r_{x,y}\big[x^{-2}y^{-2}(x-y)^{-4}\big]$ is a well-defined distribution, but their product is not.

The tactic followed in [1, 4] is to invoke Green's integration-by-parts formula to shift the Laplacian to the left and use the fundamental solution for it. Paper [2] purports instead to deal with the overall divergence "as a three-point problem". Their claim is firstly that the whole graph is renormalized by

$$(I - T_{x,y,0})(I - T_{x,0})x^{-2}y^{-2}(x-y)^{-4}.$$

Secondly, that the handy and correct formula

$$A(\Delta B) = (\Delta A)B + \partial_\beta(A\partial_\beta B - B\partial_\beta A), \tag{4}$$

employed in [1] and borrowed by [4], is not to be used, on the grounds that such a trick reverts to a two-point problem, while they want to grapple directly with the three-point problem. Thirdly, that the singular behaviors of $r_{x,y}\big[x^{-2}y^{-2}(x-y)^{-4}\big]$ and of $-2\pi^2\,\delta(y)\,x^{-4}\log|x|/l$ are the same.

Again, the mathematical argument there given for all that is hard to bear. However, the last assertion is correct, and it can be made sense of as follows. Note that

$$\Big\langle x^{-2}z^{-2}\,\Delta\Big((x-z)^{-2}\log\frac{|x-z|}{l}\Big), \varphi(x,z)\Big\rangle$$

$$= \Big\langle x^{-2}z^{-2}\,\Delta\Big((x-z)^{-2}\log\frac{|x-z|}{l}\Big), \varphi(x,0)\Big\rangle$$
$$+ \Big\langle x^{-2}y^{-2}\,\Delta\Big((x-y)^{-2}\log\frac{|x-y|}{l}\Big), \varphi(x,y)-\varphi(x,0)\Big\rangle .$$

The second integral is finite, and the first one is proportional to

$$\langle \delta(y)\, x^{-4}\log|x|/l, \varphi(x,y)\rangle .$$

In practice we are back to the two-point problem. A similar argument works whenever the graph has been rendered "primitive" by partial renormalization. The authors of [2] continue their exposition as follows. In DiffRen one has

$$r_{x,0}\big[x^{-4}\log|x|/l\big] = -\frac{1}{4}\,\Delta\frac{\log^2|x|/l+\log|x|/l}{x^2} .$$

Therefore they write:

$$r_{x,y,0}\big[r_{x,0}[x^{-2}y^{-2}(x-y)^{-4}]\big] = -\frac{1}{2}\,x^{-2}y^{-2}\,\Delta\big((x-y)^{-2}\log|x-y|/l\big)$$
$$-\,2\pi^2\,\delta(y)x^{-4}\log|x|/l - \frac{\pi^2}{2}\,\delta(y)\,\Delta\frac{\log^2|x|/l+\log|x|/l}{x^2} ,$$

with the contention that, although neither of the first two terms in the last expression exists *strictu sensu*, their combination is a well-defined distribution. The situation is then clarified by use of (4) nevertheless, whereby the second term in the above display completely drops out, and we are left with the third one plus a well-defined divergence—in the sense of vector calculus, see right below.

With our method, there comes

$$-\frac{1}{2}\,x^{-2}y^{-2}\,\Delta_y\Big((x-y)^{-2}\log\frac{|x-y|}{l}\Big)$$
$$= 2\pi^2\,\delta(y)x^{-4}\log\frac{|x|}{l} + \frac{1}{2}\,x^{-2}\,\partial_y^\beta L_\beta(x-y;y),$$

where

$$L_\beta(x-y;y) := (x-y)^{-2}\log\frac{|x-y|}{l}\,\partial^y_\beta y^{-2} - y^{-2}\,\partial^y_\beta\Big((x-y)^{-2}\log\frac{|x-y|}{l}\Big).$$

Moreover, the term $2\pi^2\,\delta(y)x^{-4}\log|x|/l$ in our treatment, as done already in (3), is renormalized according to [4, Eq. A.4]:

$$2\pi^2 R_{x,y,0}[x^{-4}\log|x|/l\,\delta(y)] = -\frac{\pi^2}{2}\,\delta(y)\,\Delta\frac{\log^2|x|/l+\log|x|/l}{x^2} + \pi^4\,\delta(x)\,\delta(y).$$

Finally, we ought to contend with the last term in (3):

$$R_{x,y,0}[\pi^2 x^{-4}\,\delta(x-y)] = -\frac{\pi^2}{2}\,\Delta\frac{\log|x|/l}{x^2}\,\delta(x-y) + \pi^4\,\delta(x)\,\delta(y).$$

In summary, with obvious abbreviated notations:

$$R_{x,y,0}\,\bigtriangledown\,(x,y) = \frac{1}{2}x^{-2}\,\partial_y^\beta L_\beta(x-y;y) - \frac{\pi^2}{2}\,\delta(y)\,\Delta\frac{\log^2|x|/l + \log|x|/l}{x^2}$$
$$- \frac{\pi^2}{2}\,\Delta\frac{\log|x|/l}{x^2}\,\delta(x-y) + 2\pi^4\,\delta(x)\,\delta(y);$$
$$r_{x,y,0}\,\bigtriangledown\,(x,y) = \frac{1}{2}x^{-2}\,\partial_y^\beta L_\beta(x-y;y) - \frac{\pi^2}{2}\,\delta(y)\,\Delta\frac{\log^2|x|/l + \log|x|/l}{x^2}.$$

We remark that the differences between DiffRen and the improved Epstein–Glaser method are of no consequence for the β-function, up to third order in the coupling constant [4, Sect. 6].

Note that we may as well symmetrize:

$$r_{x,y,0}\,\bigtriangledown\,(x,y) = \frac{1}{4}x^{-2}\,\partial_y^\beta L_\beta(x-y;y) - \frac{\pi^2}{4}\,\delta(y)\,\Delta\frac{\log^2|x|/l + \log|x|/l}{x^2}$$
$$+ \frac{1}{4}y^{-2}\,\partial_y^\beta L_\beta(x-y;x) - \frac{\pi^2}{4}\,\delta(x)\,\Delta\frac{\log^2|y|/l + \log|y|/l}{y^2}.$$

4 More General Procedures

It is plausibly claimed in [2] that more complicated graphs can be tackled by the systematics of the Bogoliubov recursion, or its descendant the . That is,

$$R\Gamma = (I - T_\Gamma)\bar{R}_\Gamma, \tag{5}$$

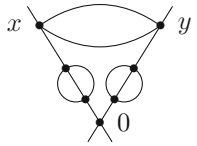
where the $\bar{R}_\Gamma$ object, renormalized but for the overall divergence is given by:

$$\bar{R}_\Gamma = I + \sum_{\mathcal{P}}\prod_{v\in\mathcal{P}}(-T_v\bar{R}v)\prod\prod \text{prop}, \tag{6}$$

where the sum is over the partitions of Γ into divergent generalized vertices v, and $\prod\prod$ prop denotes the product of propagators corresponding to all lines which connect the different elements of the partition.

The notational contortions above are again clear, but we do not take issue with them; rather we hasten to revisit a definitely amusing example. We ponder the six-loop graph Γ obtained when one "stye" develops on each of the single propagators

in a winecup graph:



Our authors claim that, after dealing with the subdivergences, the partially renormalized graph comes out as

$$r_{x,y}\Gamma \propto \frac{\log|x|/l}{x^2}\,\frac{\log|y|/l}{y^2}\,\Delta\frac{\log|x-y|/l}{(x-y)^2}\,; \tag{7}$$

and they set out to cure the overall divergence of the graph as $x, y \to 0$. Our method sustains their claim: each of the "dressed propagator" amplitudes for this diagram are of the form, with obvious labels:

$$\iint r_{x,0}\big[v^{-2}(v-w)^{-6}(w-x)^{-2}\big]\,dv\,dw = \iint r_{x,0}\big[v^{-2}u^{-6}(v-u-x)^{-2}\big]\,du\,dv.$$

Notice that this is a nested convolution; the inner integral is of the form $R[r^{-6}]*r^{-2}$, which exists by the theory of [4, Sect. 3]. As long as convolution can be effected, rule (2) proceeds without obstruction.

The displayed integral becomes

$$-\frac{1}{16}\iint v^{-2}(v-u-x)^{-2}\Big(\Delta^2\Big(u^{-2}\log\frac{|u|}{l}\Big)-5\pi^2\,\Delta\delta(u)\Big)\,dv\,du.$$

On integrating by parts and dropping total derivatives in the integrals over internal vertices, we then obtain

$$\begin{aligned}
&\frac{\pi^2}{4}\iint v^{-2}\Big(\Delta\Big(u^{-2}\log\frac{|u|}{l}\Big)-5\pi^2\,\delta(u)\Big)\,\delta(v-u-x)\,dv\,du\\
&\quad=\frac{\pi^2}{4}\int (u+x)^{-2}\Big(\Delta\Big(u^{-2}\log\frac{|u|}{l}\Big)-5\pi^2\,\delta(u)\Big)\,du\\
&\quad=-\pi^4\int u^{-2}\log\frac{|u|}{l}\,\delta(u+x)\,du-\frac{5\pi^4}{4}\,x^{-2}=-\pi^4x^{-2}\Big(\log\frac{|x|}{l}+\frac{5}{4}\Big),
\end{aligned}$$

where the extra term with respect to formula (7) is due to our different treatment of the basic "sunset" self-energy diagram: as usual we define it so that

$$x^2R_{x,0}[x^{-6}] = R_{x,0}[x^{-4}],$$

which fails for DiffRen.

Therefore we have to renormalize the overall divergence

$$\pi^8\Big(\frac{\log|x|/l}{x^2}\,\frac{\log|y|/l}{y^2}+\frac{5}{4}x^{-2}\frac{\log|y|/l}{y^2}+\frac{5}{4}y^{-2}\frac{\log|x|/l}{x^2}+\frac{25}{16}x^{-2}y^{-2}\Big)$$
$$\times\Big(-\frac{1}{2}\,\Delta\Big((x-y)^{-2}\log\frac{|x-y|}{l}\Big)+\pi^2\,\delta(x-y)\Big).$$

Several of the terms above bring nothing new; we concentrate on the most difficult one, of the form (7), the only one recognized in [2]. Its authors argue that as $x\sim y\sim 0$ one has:

$$r_{x,y}\Gamma\sim -32\pi^2\,\delta(y)\,\frac{\log^3|x|/l}{x^4}\,, \tag{8}$$

which they renormalize by DiffRen as

$$4\pi^2\,\delta(y)\,\Delta\frac{\log^4|x|/l+2\log^3|x|/l+3\log^2|x|/l+3\log|x|/l}{x^2}\,. \tag{9}$$

We pause to point to our essentially coincident formula [4, A.2]:

$$R_{x,0}\,\frac{\log^3|x|/l}{x^4}$$
$$=-\frac{1}{8}\,\Delta\frac{\log^4|x|/l+2\log^3|x|/l+3\log^2|x|/l+3\log|x|/l}{x^2}+\frac{3}{4}\,\pi^2\,\delta(x).$$

Of course, the expression resulting from (8) and (9):

$$\frac{\log|x|/l}{x^2}\,\frac{\log|y|/l}{y^2}\,\Delta\frac{\log|x-y|/l}{(x-y)^2}+4\pi^2\,\delta(y)\Big[\frac{8\log^3|x|/l}{x^4}$$
$$+\,\Delta\frac{\log^4|x|/l+2\log^3|x|/l+3\log^2|x|/l+3\log|x|/l}{x^2}\Big]$$

is rather ugly, since the first two terms are undefined. However, they cleverly add and subtract to it $y^{-2}x^{-2}\log|x|/l\,\Delta\big((x-y)^{-2}\log|x-y|/l\big)$, and applying Green's formula, everything is rewritten:

$$\frac{\log|x|/l}{x^2}\,\frac{\log|y|/l}{y^2}\,\Delta\frac{\log|x-y|/l}{(x-y)^2}\longmapsto\frac{\log|x|/l}{x^2}\,\frac{\log|y|/|x|}{y^2}\,\Delta\frac{\log|x-y|/l}{(x-y)^2}$$
$$+\,\frac{\pi^2}{2}\,\delta(y)\Big[\Delta\frac{\log^4|x|/l+2\log^3|x|/l+3\log^2|x|/l+3\log|x|/l}{x^2}\Big]$$
$$-\,\frac{\log^2|x|/l}{x^2}\,\partial_y^\beta L_\beta(x-y;y).$$

The way to improve on this is symmetrization:

$$r_{x,y,0}r_{x,y}\Gamma = \frac{\pi^2}{2}\,\delta(y)\left[\Delta\frac{\log^4|x|/l + 2\log^3|x|/l + 3\log^2|x|/l + 3\log|x|/l}{x^2}\right]$$
$$+ \frac{\pi^2}{2}\,\delta(x)\left[\Delta\frac{\log^4|y|/l + 2\log^3|y|/l + 3\log^2|y|/l + 3\log|y|/l}{y^2}\right]$$
$$- \frac{\log^2|x|/l}{x^2}\,\partial_y^\beta L_\beta(x-y;y) - \frac{\log^2|y|/l}{y^2}\,\partial_x^\beta L_\beta(y-x;x).$$

The task of computing the remaining terms in $R_{x,y,0}R_{x,y}\,\Gamma$ is comparatively easier. The ones containing the factor $\delta(x-y)$ simply go into

$$\pi^{10}\delta(x-y)\left[R_{x,0}\,\frac{\log^2|x|/l}{x^4} + \frac{5}{2}\,R_{x,0}\,\frac{\log|x|/l}{x^4} + \frac{25}{16}\,R_{x,0}\,\frac{1}{x^4}\right],$$

in terms of known renormalized expressions [4]. Of the three remaining terms, two are totally similar:

$$-\frac{5}{8}\Big(x^{-2}\,\frac{\log|y|/l}{y^2} + y^{-2}\,\frac{\log|x|/l}{x^2}\Big)\Delta\Big((x-y)^{-2}\log\frac{|x-y|}{l}\Big),$$

and can be computed as above by Green's formula, and the other is of the same form as the winecup graph.

5 Conclusion

Formulae (5) and (6) work like guiding principles, rather than calculational recipes. Actual production of closed formulas relies on a bag of tricks. While the application of the inductive principle of [4] often profits from similar tricks, it appears to be better adapted in practice to deal with complex diagrams.

Acknowledgements The author is thankful to Joseph C. Várilly for some very useful comments. His work was supported by the Spanish Ministry for Science through grant FPA2012–35453.

References

1. D.Z. Freedman, K. Johnson, J.I. Latorre, Differential regularization and renormalization: a new method of calculation in quantum field theory. Nucl. Phys. B **371**, 352–414 (1992)
2. J.I. Latorre, C. Manuel, X. Vilasís-Cardona, Systematic differential renormalization at all orders. Ann. Phys. **231**, 149–173 (1994)

3. N.M. Nikolov, R. Stora, I. Todorov, Renormalization of massless Feynman amplitudes in configuration space. Rev. Math. Phys. **26**, 1430002 (2014)
4. J.M. Gracia-Bondía, H. Gutiérrez, J.C. Várilly, Improved Epstein–Glaser renormalization in x-space versus differential renormalization. Nucl. Phys. B **886**, 824–869 (2014)
5. M. Dütsch, K. Fredenhagen, K.J. Keller, K. Rejzner, Dimensional regularization in position space, and a forest formula for Epstein–Glaser renormalization. J. Math. Phys. **55**, 122303 (2014)
6. H. Epstein, V. Glaser, The role of locality in perturbation theory. Ann. Inst. Henri Poincaré A **19**, 211–295 (1973)
7. S. Weinberg, High-energy behavior in quantum field theory. Phys. Rev. **118**, 838–849 (1980)
8. E.B. Manoukian, *Renormalization* (Academic Press, London, 1983)
9. R. Stora, in *Fifty years of Yang–Mills Theory*, ed. by G. 't Hooft (World Scientific, Singapore, 2005), pp. 137–167
10. J.M. Gracia-Bondía, Improved Epstein–Glaser renormalization in coordinate space I. Euclidean framework. Math. Phys. Anal. Geom. **6**, 59–88 (2003)
11. A.N. Kuznetsov, F.V. Tkachov, V.V. Vlasov, *Techniques of distributions in perturbative quantum field theory I.* arXiv:hep-th/9612037
12. N.N. Bogoliubov, D.V. Shirkov, *Introduction to the theory of quantized fields*, 3rd edn. (Wiley, New York, 1980)

Higgs Mechanism and Renormalization Group Flow: Are They Compatible?

Michael Dütsch

Contents

Abstract Usually, the Lagrangian of a model for massive vector bosons is derived in a geometric way by the Higgs mechanism. We investigate whether this geometric structure is maintained under the renormalization group (RG) flow. Using the framework of Epstein-Glaser renormalization, we find that the answer is 'no', if the renormalization mass scale(s) are chosen in a way corresponding to the minimal subtraction scheme. This result is derived for the $U(1)$-Higgs model to 1-loop order. On the other hand we give a model-independent proof that physical consistency, which is a weak form of BRST-invariance of the time-ordered products, is stable under the RG-flow.

Keywords Perturbative quantum gauge theories • Epstein-Glaser renormalization • Higgs mechanism • Renormalization group flow

M. Dütsch (✉)
Institut für Theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany
e-mail: michael.duetsch@theorie.physik.uni-goe.de

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_4

Mathematics Subject Classification (2010). Primary 81T15; Secondary 81T13, 81T17

1 Introduction

By the renormalization group (RG) flow we have a tool to describe a QFT-model at different scales. In this description, the basic fields, the gauge-fixing parameter, the masses and the prefactors of the various interaction terms are scale-dependent quantities.

On the other hand, the derivation of the Lagrangian of a model for massive vector bosons by the Higgs mechanism, i.e. by spontaneous symmetry breaking of a gauge theory, implies that the prefactors of the various interaction terms are uniquely determined functions of the coupling constant(s) and masses.

Do these functions remain unchanged under the RG-flow, i.e. under an arbitrary change of scale? This question is a reformulation of the title of this paper. Since the non-trivial contributions to the RG-flow come from loop diagrams and different interaction terms get different loop-corrections, it is uncertain, whether the answer is 'yes'. Or – one can come to the same conclusion by considering the underlying frameworks: the Higgs mechanism is formulated in classical field theory and, to the best of our knowledge, it is not understood in a pure QFT framework; on the other hand, the RG-flow is a pure quantum effect.

Some readers may wonder whether the Lagrangian of the scaled model still describes a consistent QFT-model, if it is not derivable by the Higgs mechanism? The answer is 'yes', for the following reasons: by Poincaré invariance, relevant discrete symmetries and renormalizability are maintained under the RG-flow, the crucial requirement for consistency of a quantum gauge model is physical consistency (PC) [8, 17]. This is the condition that the free BRST-charge[1] commutes with the "S-matrix" in the adiabatic limit, in order that the latter induces a well-defined operator on the physical subspace. We give a model-independent proof that PC is maintained under the RG-flow (Theorem 3.1).

In the literature we could not find an explicit 'yes' or 'no' to the question in the title. However, some papers silently assume that the answer is 'yes' – see the few examples mentioned in [5, Introduction]. The answer certainly depends on the renormalization scheme.

We work with the definition of the RG-flow given in framework Epstein-Glaser renormalization [12]: since a scaling transformation amounts to a change of the renormalization prescription, it can equivalently be expressed by a renormalization of the interaction – this is an application of the Main Theorem, see [3, 6, 15, 18]. The so defined RG-flow depends on the renormalization scheme via the two possibilities

[1] That is the charge implementing the BRST-transformation of the asymptotic free fields.

that the scaling transformation may act on the renormalization mass scale(s) or it may not; and this may be different for different Feynman diagrams.

We investigate the question in the title by explicit 1-loop calculations – the technical details are omitted in this paper, they are given in [5]. To minimise the computations, we study the model of one massive vector field, that is, we start the RG-flow with the $U(1)$-Higgs model.

2 Precise Formulation of the Question

Lagrangian of the initial model The just mentioned model has one massive vector field A^μ, the corresponding Stückelberg field B, a further real scalar field φ ("Higgs field") and the Fadeev-Popov ghost fields $(u\,,\,\tilde{u})$. The Lagrangian reads

$$L_{\text{total}} \simeq -\frac{1}{4}F^2 + \frac{1}{2}(D^\mu\Phi)^* D_\mu\Phi - V(\Phi) + L_{\text{gf}} + L_{\text{ghost}}\,, \tag{1}$$

where $\simeq$ means equal up to the addition of terms of type $\partial^a A$, where $|a| \geq 1$ and A is a local field polynomial. In addition we use the notations $F^2 := (\partial^\mu A^\nu - \partial^\nu A^\mu)(\partial_\mu A_\nu - \partial_\nu A_\mu)$,

$$\Phi := iB + \frac{m}{\kappa} + \varphi\,, \quad D^\mu := \partial^\mu - i\kappa\, A^\mu \tag{2}$$

and

$$V(\Phi) := \frac{\kappa^2 m_H^2}{8m^2}(\Phi^*\Phi)^2 - \frac{m_H^2}{4}(\Phi^*\Phi) + \frac{m_H^2 m^2}{8\kappa^2}\,, \tag{3}$$

where κ is the coupling constant and m and m_H are the masses of the A- and φ-field, respectively, as it turns out below in (6). The gauge-fixing and ghost Lagrangian are given by

$$L_{\text{gf}} := -\frac{\Lambda}{2}\left(\partial A + \frac{m}{\Lambda}B\right)^2 \tag{4}$$

and

$$L_{\text{ghost}} := \partial\tilde{u}\partial u - \frac{m^2}{\Lambda}\tilde{u}u - \frac{\kappa\, m}{\Lambda}\tilde{u}u\varphi\,, \tag{5}$$

respectively, where Λ is the gauge-fixing parameter. The masses of the A- and φ-field are generated by the Higgs mechanism.

In view of perturbation theory we split L_{total} into a free part L_0 (all bilinear terms) and an interacting part L (all tri- and quadrilinear terms):

$$\begin{aligned} L_0 &= -\frac{1}{4}F^2 + \frac{m^2}{2}A^2 + \frac{1}{2}(\partial B)^2 - \frac{m^2}{2\Lambda}B^2 - \frac{\Lambda}{2}(\partial A)^2 \\ &\quad + \frac{1}{2}(\partial\varphi)^2 - \frac{m_H^2}{2}\varphi^2 + \partial\tilde{u}\partial u - \frac{m^2}{\Lambda}\tilde{u}u\,, \end{aligned} \tag{6}$$

$$\begin{aligned} L &= \kappa\Big(mA^2\varphi - \frac{m^2}{\Lambda}\tilde{u}u\varphi + B(A\partial\varphi) - \varphi(A\partial B) - \frac{m_H^2}{2m}\varphi^3 - \frac{m_H^2}{2m}B^2\varphi\Big) \\ &\quad + \kappa^2\Big(\frac{1}{2}A^2(\varphi^2+B^2) - \frac{m_H^2}{8m^2}\varphi^4 - \frac{m_H^2}{4m^2}\varphi^2B^2 - \frac{m_H^2}{8m^2}B^4\Big)\,, \end{aligned} \tag{7}$$

where $V^2 := V^\mu V_\mu$, $VW := V^\mu W_\mu$ for Lorentz vectors $V, W \in \mathbb{C}^4$.

Remark 2.1 The BRST-transformation is a graded derivation which commutes with partial derivatives and is given on the basic fields by

$$\begin{gathered} sA^\mu = \partial^\mu u\,, \quad sB = mu + \kappa\, u\varphi\,, \quad s\varphi = -\kappa\, Bu\,, \\ su = 0\,, \quad s\tilde{u} = -\Lambda\,(\partial A + \frac{m}{\Lambda}B)\,. \end{gathered} \tag{8}$$

With $s_0 := s|_{\kappa=0}$ we denote its version for the free theory. We point out that L and L_0 are invariant w.r.t. the pertinent BRST-transformation:

$$sL \simeq 0\,, \qquad s_0L_0 \simeq 0\,, \tag{9}$$

where $\simeq$ has the same meaning as above.

Definition of the RG-flow In view of Epstein-Glaser renormalization [12] we write

$$L = \kappa\, L_1 + \kappa^2\, L_2 \tag{10}$$

and introduce an adiabatic switching of the coupling constant by a test function $g \in \mathcal{D}(\mathbb{R}^4)$:

$$L(g) \equiv L^{\mathbf{m}}(g) := \int dx\,\Big(\kappa\, g(x)\, L_1(x) + \big(\kappa\, g(x)\big)^2\, L_2(x)\Big)\,. \tag{11}$$

For later purpose we have introduced the upper index $\mathbf{m} := (m, m_H)$.

In the Epstein-Glaser framework the RG-flow is defined by a scaling transformation σ_ρ [3, 6, 15]:

$$\sigma_\rho^{-1}(\phi(x)) = \rho\,\phi(\rho x)\,, \quad \phi = A^\mu, B, \varphi, u, \tilde{u}\,, \quad \rho > 0\,, \tag{12}$$

and a simultaneous scaling of the masses $\mathbf{m} \mapsto \rho^{-1}\mathbf{m} = (\rho^{-1}m, \rho^{-1}m_H)$; see [6] for the precise definition of σ_ρ. Under this transformation the classical action is invariant (up to a scaling of the switching function g).

In QFT scaling invariance is in general broken in the process of renormalization. To explain this, we introduce the generating functional $S(iL(g))$ of the time-ordered products of $L(g)$, i.e.

$$T_n(L(g)^{\otimes n}) = \frac{d^n}{i^n\, d\eta^n}|_{\eta=0}\, S(i\eta\, L(g)) \quad \text{or generally} \quad T_n = S^{(n)}(0)\,, \tag{13}$$

which we construct inductively by Epstein-Glaser renormalization [12]. To define the RG-flow, we need to perform the adiabatic limit

$$\mathbf{S}[L] := \lim_{\varepsilon\downarrow 0} S(iL(g_\varepsilon))\,, \quad g_\varepsilon(x) := g(\varepsilon x)\,, \tag{14}$$

where $g(0) = 1$ is assumed. For a purely massive model and with a suitable (re)normalization of $S(iL(g))$, this limit exists in the strong operator sense. For a rigorous proof of this statement we refer to [12, 13]; in this paper we treat the adiabatic limit on a heuristic level.

The Main Theorem of perturbative renormalization [6, 15, 18] implies that a scaling transformation of $\mathbf{S}[L]$, i.e.

$$\mathbf{S}_{\mathbf{m}}[L^{\mathbf{m}}] \mapsto \sigma_\rho(\mathbf{S}_{\rho^{-1}\mathbf{m}}[\sigma_\rho^{-1}(L^{\mathbf{m}})])\,,$$

can equivalently be expressed by a renormalization of the interaction $L^{\mathbf{m}} \mapsto z_\rho(L^{\mathbf{m}})$ ("running interaction"), explicitly

$$\sigma_\rho(\mathbf{S}_{\rho^{-1}\mathbf{m}}[\sigma_\rho^{-1}(L^{\mathbf{m}})]) = \mathbf{S}_{\mathbf{m}}[z_\rho(L^{\mathbf{m}})]\,, \tag{15}$$

where the lower index $\mathbf{m}$ of $\mathbf{S}_{\mathbf{m}}$ denotes the masses of the Feynman propagators. This is explained in detail in Sect. 3.

The form of the running interaction Using general properties of the running interaction (derived in [6]), we know that each term appearing in $z_\rho(L)$ is Lorentz invariant, has ghost number $= 0$ and has mass dimension ≤ 4. In addition, using that L (7) is even under the field parity transformation

$$(A, B, \varphi, u, \tilde{u}) \mapsto (-A, -B, \varphi, u, \tilde{u})\,, \tag{16}$$

one easily derives that also $z_\rho(L)$ is even under this transformation. One can also show that only one term containing the Fadeev-Popov ghosts can appear in $(z_\rho(L) - L)$, namely a term $\sim \tilde{u}u$. Moreover, with a slight restriction on the (re)normalization of $S(iL(g))$, one can exclude 1-leg terms from $z_\rho(L)$ [5].

Using these facts, we conclude that the running interaction has the form

$$\begin{aligned} z_\rho(L) \simeq & \hbar^{-1}\Big[k_\rho - \frac{1}{4}a_{0\rho}\,F^2 + \frac{m^2}{2}a_{1\rho}A^2 - \frac{a_{2\rho}}{2}(\partial A)^2 + \frac{1}{2}b_{0\rho}(\partial B)^2 - \frac{m^2}{2\,\Lambda}\,b_{1\rho}\,B^2 \\ & + \frac{1}{2}c_{0\rho}\,(\partial\varphi)^2 - \frac{m_H^2}{2}c_{1\rho}\,\varphi^2 - \frac{m^2}{\Lambda}\,c_{2\rho}\,\tilde{u}u + b_{2\rho}\,m\,(A\partial B) \\ & + \kappa\Big((1+l_{0\rho})\,m\,A^2\varphi - \frac{m}{\Lambda}\,\tilde{u}u\varphi + (1+l_{1\rho})\,B(A\partial\varphi) \\ & - (1+l_{2\rho})\,\varphi(A\partial B) - \frac{(1+l_{3\rho})m_H^2}{2m}\,\varphi^3 - \frac{(1+l_{4\rho})m_H^2}{2m}\,B^2\varphi\Big) \\ & + \kappa^2\Big(\frac{(1+l_{5\rho})}{2}A^2\,\varphi^2 + \frac{(1+l_{6\rho})}{2}A^2\,B^2 - \frac{(1+l_{7\rho})m_H^2}{8m^2}\,\varphi^4 \\ & - \frac{(1+l_{8\rho})m_H^2}{4m^2}\,\varphi^2 B^2 - \frac{(1+l_{9\rho})m_H^2}{8m^2}\,B^4 + l_{11\rho}\,(A^2)^2\Big)\Big]\,, \end{aligned} \tag{17}$$

where $\simeq$ has the same meaning as in (1) and $k_\rho \in \hbar\,\mathbb{C}[[\hbar]]$ is a constant field (it is the contribution of the vacuum diagrams), which may be neglected.

The dimensionless, ρ-dependent coefficients k_ρ, $a_{j\rho}$, $b_{j\rho}$, $c_{j\rho}$ and $l_{j\rho}$ will collectively be denoted by e_ρ. In principle these coefficients are computable – at least to lowest orders; however, at the present stage they are unknown. As shown in [5], the e_ρ's are formal power series in $\kappa^2\hbar$ with vanishing term of zeroth order,

$$e_\rho = \sum_{n=1}^{\infty} e_\rho^{(n)}\,(\kappa^2\hbar)^n\,, \quad e = k, a_j, b_j, c_j, l_j\,. \tag{18}$$

Due to $z_{\rho=1}(L) = L/\hbar$, all functions $\rho \mapsto e_\rho$ have the initial value 0 at $\rho = 1$.

Renormalization of the wave functions, masses, gauge-fixing parameter and coupling parameters Except for the $A\partial B$- and A^4-term, all field monomials appearing in $z_\rho(L)$ are already present in $L_0 + L$. Therefore, introducing new fields, which are of the form

$$\phi_\rho(x) = f_\phi(\rho)\,\phi(x)\,, \quad \phi = A,\, B,\, \varphi, \tag{19}$$

where $f_\phi : (0,\infty) \to \mathbb{C}$ is a ϕ-dependent function, and introducing a running gauge-fixing parameter Λ_ρ, running masses $\mathbf{m}_\rho \equiv (m_\rho, m_{B\rho}, m_{u\rho}, m_{H\rho})$ and running coupling constants $\kappa_\rho\lambda_{j\rho}$, we can achieve that $L_0 + z_\rho(L) - k_\rho$ has roughly the same form as $L_0 + L$:

$$L_0 + z_\rho(L) - k_\rho = L_0^\rho + L^\rho\,, \tag{20}$$

where

$$L_0^\rho = -\frac{1}{4}F_\rho^2 + \frac{m_\rho^2}{2}A_\rho^2 + \frac{1}{2}(\partial B_\rho)^2 - \frac{m_{B\rho}^2}{2}B_\rho^2 - \frac{\Lambda_\rho}{2}(\partial A_\rho)^2 + \frac{1}{2}(\partial\varphi_\rho)^2 - \frac{m_{H\rho}^2}{2}\varphi_\rho^2 + \partial\tilde{u}\partial u - m_{u\rho}^2\tilde{u}u\,, \tag{21}$$

(with $F_\rho^{\mu\nu} := \partial^\mu A_\rho^\nu - \partial^\nu A_\rho^\mu$) and

$$\begin{aligned} L^\rho = \kappa_\rho\Big(& m_\rho A_\rho^2\varphi_\rho - \frac{\lambda_{10\rho}\,m_{u\rho}^2}{m_\rho}\tilde{u}u\varphi + \lambda_{1\rho}B_\rho(A_\rho\partial\varphi_\rho) \\ & - \lambda_{2\rho}\varphi_\rho(A_\rho\partial B_\rho) - \frac{\lambda_{3\rho}m_{H\rho}^2}{2m_\rho}\varphi_\rho^3 - \frac{\lambda_{4\rho}m_{H\rho}^2}{2m_\rho}B_\rho^2\varphi_\rho\Big) \\ & + \kappa^2\Big(\frac{\lambda_{5\rho}}{2}A_\rho^2\varphi_\rho^2 + \frac{\lambda_{6\rho}}{2}A_\rho^2B_\rho^2 - \frac{\lambda_{7\rho}m_{H\rho}^2}{8m_\rho^2}\varphi_\rho^4 \\ & - \frac{\lambda_{8\rho}m_{H\rho}^2}{4m_\rho^2}\varphi_\rho^2B_\rho^2 - \frac{\lambda_{9\rho}m_{H\rho}^2}{8m_\rho^2}B_\rho^4 + \lambda_{11\rho}A_\rho^2\Big) \\ & + \big((\lambda_{12\rho}-1)m_\rho + \sqrt{\Lambda_\rho}\,m_{B\rho}\big)A_\rho\partial B_\rho\,. \end{aligned} \tag{22}$$

In view of the Higgs mechanism for $L + z_\rho(L)$ (27), the definition of $\lambda_{12\rho}$ is rather complicated. Apart from the $A\partial B$-term, we have absorbed the novel bilinear interaction terms in the free Lagrangian. Since every new field is of the form (19), the condition (20) is an equation for polynomials in the old fields; equating the coefficients we obtain the following explicit formulas for the running quantities:

– for the wave functions

$$A_\rho^\mu = \sqrt{1+a_{0\rho}}\,A^\mu\,, \quad B_\rho = \sqrt{1+b_{0\rho}}\,B\,, \quad \varphi_\rho = \sqrt{1+c_{0\rho}}\,\varphi\,; \tag{23}$$

– for the gauge-fixing parameter

$$\Lambda_\rho = \frac{\Lambda + a_{2\rho}}{1+a_{0\rho}}\,; \tag{24}$$

– for the masses

$$\begin{aligned} m_\rho &= \sqrt{\frac{1+a_{1\rho}}{1+a_{0\rho}}}\,m\,, & m_{H\rho} &= \sqrt{\frac{1+c_{1\rho}}{1+c_{0\rho}}}\,m_H\,, \\ m_{B\rho} &= \sqrt{\frac{1+b_{1\rho}}{1+b_{0\rho}}}\,\frac{m}{\sqrt{\Lambda}}\,, & m_{u\rho} &= \sqrt{1+c_{2\rho}}\,\frac{m}{\sqrt{\Lambda}}\,; \end{aligned} \tag{25}$$

– for the coupling constant

$$\kappa_\rho = \frac{1 + l_{0\rho}}{\sqrt{(1 + a_{0\rho})(1 + a_{1\rho})(1 + c_{0\rho})}}\,\kappa\,; \tag{26}$$

and the running coupling parameters $\lambda_{j\rho}$ are determined analogously.

By the renormalization of the wave functions, masses and gauge fixing-parameter, we change the splitting of the total Lagrangian $L_0 + z_\rho(L)$ into a free and interacting part, i.e. we change the starting point for the perturbative expansion. To justify this, one has to show that the two perturbative QFTs given by the splittings $L_0 + z_\rho(L)$ and $L_0^\rho + L^\rho$, respectively, have the same physical content.[2] Using the framework of algebraic QFT, one has to show the following: given a renormalization prescription for $L_0 + z_\rho(L)$, there exists a renormalization prescription for $L_0^\rho + L^\rho$, such that, in the algebraic adiabatic limit, the pertinent nets of local observables (see [2] or [3, 6]) are equivalent. This task is beyond the scope of this paper.

Higgs mechanism at an arbitrary scale Our main question is whether the Lagrangian $L_0^\rho + L^\rho$ can also be derived by the Higgs mechanism for all $\rho > 0$. By the latter we mean

$$L_0^\rho + L^\rho \simeq -\frac{1}{4}F_\rho^2 + \frac{1}{2}(D_\rho^\mu \Phi_\rho)^* D_{\rho\mu}\Phi_\rho - V_\rho(\Phi_\rho) + L_{\mathrm{gf}}^\rho + L_{\mathrm{ghost}}^\rho\,, \tag{27}$$

where Φ_ρ, D_ρ and $V_\rho(\Phi_\rho)$ are obtained from (2) to (3) by replacing $(A^\mu, B, \varphi, m, m_H, \Lambda)$ by $(A_\rho^\mu, B_\rho, \varphi_\rho, m_\rho, m_{H\rho}, \Lambda_\rho)$ and

$$\begin{aligned} L_{\mathrm{gf}}^\rho &:= -\frac{\Lambda_\rho}{2}\left(\partial A_\rho + \frac{m_{B\rho}}{\sqrt{\Lambda_\rho}}B_\rho\right)^2, \\ L_{\mathrm{ghost}}^\rho &:= \partial\tilde{u}\cdot\partial u - m_{u\rho}^2\,\tilde{u}u - \frac{\kappa_\rho\,\lambda_{10\rho}\,m_{u\rho}^2}{m_\rho}\,\tilde{u}u\varphi_\rho\,. \end{aligned} \tag{28}$$

For the property (27) we also say that the model "can be geometrically interpreted as a spontaneously broken gauge theory at all scales" [5]. By a straightforward calculation we find that (27) is equivalent to

$$\lambda_{1\rho} = \lambda_{2\rho} = \ldots = \lambda_{9\rho} = 1\,, \quad \lambda_{11\rho} = \lambda_{12\rho} = 0\,. \tag{29}$$

To simplify the calculations we assume that initially we are in Feynman gauge: $\Lambda_{\rho=1} = 1$. With that the geometrical interpretability (29) is equivalent to the

[2] This statement can be viewed as an application of the "Principle of Perturbative Agreement" of Hollands and Wald [16].

following relations among the coefficients e_ρ:

$$\lambda_{1\rho} = 1 \text{ gives} \qquad \frac{1 + l_{1\rho}}{1 + l_{0\rho}} = \sqrt{\frac{1 + b_{0\rho}}{1 + a_{1\rho}}}\,, \tag{30}$$

$$\lambda_{2\rho} = 1 \text{ gives} \qquad l_{2\rho} = l_{1\rho}\,, \tag{31}$$

$$\lambda_{3\rho} = 1 \text{ gives} \qquad \frac{1 + l_{3\rho}}{1 + l_{0\rho}} = \frac{1 + c_{1\rho}}{1 + a_{1\rho}}\,, \tag{32}$$

$$\lambda_{4\rho} = 1 \text{ gives} \qquad \frac{1 + l_{4\rho}}{1 + l_{3\rho}} = \frac{1 + b_{0\rho}}{1 + c_{0\rho}}\,, \tag{33}$$

$$\lambda_{5\rho} = 1 \text{ gives} \qquad \frac{1 + l_{5\rho}}{(1 + l_{0\rho})^2} = \frac{1}{1 + a_{1\rho}}\,, \tag{34}$$

$$\lambda_{6\rho} = 1 \text{ gives} \qquad \frac{1 + l_{6\rho}}{1 + l_{5\rho}} = \frac{1 + b_{0\rho}}{1 + c_{0\rho}}\,, \tag{35}$$

$$\lambda_{7\rho} = 1 \text{ gives} \qquad \frac{1 + l_{7\rho}}{(1 + l_{0\rho})^2} = \frac{1 + c_{1\rho}}{(1 + a_{1\rho})^2}\,, \tag{36}$$

$$\lambda_{8\rho} = 1 \text{ gives} \qquad \frac{1 + l_{8\rho}}{1 + l_{7\rho}} = \frac{1 + b_{0\rho}}{1 + c_{0\rho}}\,, \tag{37}$$

$$\lambda_{9\rho} = 1 \text{ gives} \qquad \frac{1 + l_{9\rho}}{1 + l_{7\rho}} = \left(\frac{1 + b_{0\rho}}{1 + c_{0\rho}}\right)^2\,, \tag{38}$$

$$\lambda_{11\rho} = 0 \text{ gives} \qquad l_{11\rho} = 0\,, \tag{39}$$

$$\lambda_{12\rho} = 0 \text{ gives} \qquad b_{2\rho} = \sqrt{(1 + a_{2\rho})(1 + b_{1\rho})} - \sqrt{(1 + a_{1\rho})(1 + b_{0\rho})}\,. \tag{40}$$

Combining the Eqs. (32), (34) and (36) we obtain

$$\frac{1 + l_{7\rho}}{1 + l_{3\rho}} = \frac{1 + l_{5\rho}}{1 + l_{0\rho}}\,. \tag{41}$$

This condition and (40) are crucial for the geometrical interpretability, as we will see.

Remark 2.2 BRST-invariance of $L_0 + z_\rho(L)$ is a clearly stronger property than the geometrical interpretability (27). More precisely: considering the coefficients e_ρ as unknown and assuming that $s(L_0 + z_\rho(L)) \simeq 0$, we obtain rather restrictive relations among the coefficients e_ρ which imply the Eqs. (30), (31), (32), (33), (34), (35), (36), (37), (38), (39), and (40). Ignoring k_ρ, the number of coefficients e_ρ, which are left freely chosable by the BRST-property, is 3; and for the geometrical interpretability this number is 9 – see [5].

3 Physical Consistency and Perturbative Gauge Invariance

Physical consistency (PC) The generic problem of a model containing spin 1 fields is the presence of unphysical fields. A way to solve this problem in a scattering framework is to construct $S(iL(g))$ such that the following holds. For the asymptotic free fields let $\mathcal{H}_{\text{phys}}$ be the "subspace" of physical states. In the adiabatic limit $\lim g \to 1$, $S(iL(g))$ has to induce a well defined operator from $\mathcal{H}_{\text{phys}}$ into itself, which is the physically relevant S-matrix.

To formulate this condition explicitly, let Q be the generator of the free BRST-transformation $s_0 := s|_{\kappa=0}$:

$$[Q,\phi]_\star^\mp \approx i\hbar\, s_0\phi\ , \quad \phi = A^\mu\ , B\ , \varphi\ , u\ , \tilde{u}\ , \tag{42}$$

where $[\cdot\ ,\ \cdot]_\star^\mp$ denotes the graded commutator w.r.t. the $\star$-product and $\approx$ means 'equal modulo the free field equations'. With that we may write $\mathcal{H}_{\text{phys}} := \frac{\ker Q}{\operatorname{ran} Q}$, and the mentioned, fundamental condition on $S(iL(g))$ is equivalent to

$$0 \approx [Q,\mathbf{S}[L]]_\star|_{\ker Q} \equiv \lim_{\varepsilon\downarrow 0}[Q,S(iL(g_\varepsilon)/\hbar)]_\star|_{\ker Q}\ , \tag{43}$$

see [8, 17]. For simplicity we omit the restriction to $\ker Q$ and call the resulting condition "physical consistency (PC)".

Stability of PC under the RG-flow A main, model-independent result of this paper is that PC is maintained under the RG-flow.

Theorem 3.1 *Assume that $S_{\mathbf{m}}(iL(g))$ is renormalized such that the adiabatic limit $\varepsilon \downarrow 0$ exists and is unique for $\sigma_\rho \circ S_{\rho^{-1}\mathbf{m}} \circ \sigma_\rho^{-1}(iL(g_\varepsilon))\ \ \forall \rho > 0$, and such that $S_{\mathbf{m}}(iL^{\mathbf{m}}(g))$ fulfills PC for all values $m_j > 0$ of the masses $\mathbf{m} = (m_j)$. Then, the following holds:*

$$\big[Q,\mathbf{S}[z_\rho(L)]\big]_\star \equiv \lim_{\varepsilon\downarrow 0}[Q,S(iz_\rho(L)(g_\varepsilon))]_\star \approx 0\ , \quad \forall\rho > 0\ . \tag{44}$$

Hence, at least in this weak form, BRST-invariance of the time-ordered products is stable under the RG-flow.

Proof As a preparation we explain the construction of $z_\rho(L)$ and derive (15). Assuming that S fulfills the axioms of Epstein-Glaser renormalization, this holds also for the scaled time-ordered products $\sigma_\rho \circ S \circ \sigma_\rho^{-1}$; therefore, the Main Theorem [6, 15] applies: there exists a unique map $Z_\rho \equiv Z_{\rho,\mathbf{m}}$ from the space of local interactions into itself such that

$$\sigma_\rho \circ S_{\rho^{-1}\mathbf{m}} \circ \sigma_\rho^{-1} = S_{\mathbf{m}} \circ Z_{\rho,\mathbf{m}} \tag{45}$$

(the lower index $\mathbf{m}$ on S and Z_ρ denotes the masses of the underlying $\star$-product, i.e. the masses of the Feynman propagators).

In view of the adiabatic limit we investigate $Z_\rho(iL(g_\varepsilon)/\hbar)$ and take into account that $\partial g_\varepsilon(x) \sim \varepsilon$. From [6, Prop. 4.3] we know that there exist local field polynomials $p_{k\rho}(L)$ such that

$$Z_\rho(iL(g_\varepsilon)/\hbar) = \frac{i}{\hbar}\Big(L(g_\varepsilon) + \sum_{k=2}^{\infty} \int dx\; p_{k\rho}(L)(x)\,(\kappa g_\varepsilon(x))^k\Big) + \mathcal{O}(\varepsilon)\;. \tag{46}$$

Obviously, $p_{k\rho}(L)$ is not uniquely determined: one may add terms of type $\partial^a A$, $|a| \geq 1$, where A is a local field polynomial. Setting

$$z_\rho(L)(g) := \frac{1}{\hbar} \sum_{k=1}^{\infty} \int dx \left(L_k(x) + p_{k\rho}(L)(x)\right) (\kappa g(x))^k\;, \tag{47}$$

where $p_{1\rho} := 0$ and $L_k := 0$ for $k \geq 3$, we obtain

$$Z_\rho(iL(g_\varepsilon)/\hbar) = i\, z_\rho(L)(g_\varepsilon) + \mathcal{O}(\varepsilon)\;. \tag{48}$$

Using this result and (multi-)linearity of the time-ordered products, we obtain (15):

$$\begin{aligned}\sigma_\rho(\mathbf{S}_{\rho^{-1}\mathbf{m}}[\sigma_\rho^{-1}(L^{\mathbf{m}})]) &:= \lim_{\varepsilon\downarrow 0} \sigma_\rho \circ S_{\rho^{-1}\mathbf{m}} \circ \sigma_\rho^{-1}(iL^{\mathbf{m}}(g_\varepsilon)) \\ &= \lim_{\varepsilon\downarrow 0} S_{\mathbf{m}}\big(Z_\rho(iL^{\mathbf{m}}(g_\varepsilon))\big) = \lim_{\varepsilon\downarrow 0} S_{\mathbf{m}}\big(i\, z_\rho(L^{\mathbf{m}})(g_\varepsilon)\big) =: \mathbf{S}_{\mathbf{m}}[z_\rho(L^{\mathbf{m}})]\;.\end{aligned} \tag{49}$$

By assumption the limit exists on the l.h.s.; hence, it exists also on the r.h.s..

With these tools we are able to prove (44): using the relations

$$\sigma_\rho^{-1}(L^{\mathbf{m}}(g)) = L^{\rho^{-1}\mathbf{m}}(g_{1/\rho}) \qquad (\text{ again } g_\lambda(x) := g(\lambda x)\,) \tag{50}$$

and

$$\sigma_\rho(F \star_{\rho^{-1}\mathbf{m}} G) = \sigma_\rho(F) \star_{\mathbf{m}} \sigma_\rho(G)\;, \quad \rho\,\sigma_\rho \circ Q_{\rho^{-1}\mathbf{m}} = Q_{\mathbf{m}}\;, \tag{51}$$

we obtain

$$\begin{aligned}[Q_{\mathbf{m}}, S_{\mathbf{m}}(Z_\rho(iL^{\mathbf{m}}(g_\varepsilon)))]_{\star_{\mathbf{m}}} &= [Q_{\mathbf{m}}, \sigma_\rho \circ S_{\rho^{-1}\mathbf{m}}(iL^{\rho^{-1}\mathbf{m}}(g_{\varepsilon/\rho}))]_{\star_{\mathbf{m}}} \\ &= \rho\,\sigma_\rho\Big([Q_{\rho^{-1}\mathbf{m}}, S_{\rho^{-1}\mathbf{m}}(iL^{\rho^{-1}\mathbf{m}}(g_{\varepsilon/\rho}))]_{\star_{\rho^{-1}\mathbf{m}}}\Big)\;.\end{aligned} \tag{52}$$

By assumption, the adiabatic limit $\varepsilon \downarrow 0$ vanishes for the last expression. (Due to uniqueness of the adiabatic limit, it does not matter whether we perform this limit

with g or $g_{1/\rho}$.) With that and with (48) we conclude

$$0 \approx \lim_{\varepsilon\downarrow 0}[Q, S(Z_\rho(iL(g_\varepsilon)))]_\star = \lim_{\varepsilon\downarrow 0}[Q, S(i\,z_\rho(L)(g_\varepsilon))]_\star = \big[Q, \mathbf{S}[z_\rho(L)]\big]_\star\,.$$

□

Perturbative gauge invariance (PGI) For the initial model $S(iL(g))$ we admit all renormalization prescriptions which fulfill the Epstein-Glaser axioms [6, 12] and *perturbative gauge invariance (PGI)* [7, 9, 10, 19]. The latter is a somewhat stronger version of PC, which is formulated *before* the adiabatic limit $g \to 1$ is taken.

In detail, PGI is the condition that to the given interaction $L(g)$ (11) there exists a "Q-vertex"

$$\mathcal{P}^\nu(g;f) := \int dx \left(\kappa\, P_1^\nu(x) + \kappa^2 g(x)\, P_2^\nu(x)\right) f(x), \tag{53}$$

(where $g, f \in \mathcal{D}(\mathbb{R}^4)$ and P_1, P_2 are local field polynomials) and a renormalization of the time-ordered products such that

$$[Q, S\big(i\,L(g)\big)]_\star \approx \frac{d}{d\eta}|_{\eta=0}\, S\big(i\,L(g) + \eta\,\mathcal{P}^\nu(g;\partial_\nu g)\big)\,. \tag{54}$$

The latter equation is understood in the sense of formal power series in κ and $\hbar$.

That PGI implies PC, is easy to see (on the heuristic level on which we treat the adiabatic limit in this paper): the r.h.s. of (54) vanishes in the adiabatic limit, since it is linear in the Q-vertex, the latter is linear in $\partial_\nu g$ and $\partial_\nu g_\varepsilon \sim \varepsilon$.

Requiring PGI, renormalizability and some obvious properties as Poincaré invariance and relevant discrete symmetries, the Lagrangian of the Standard model of electroweak interactions has been derived in [1, 7]. In this way the presence of Higgs particles and chirality of fermionic interactions can be understood without recourse to any geometrical or group theoretical concepts (see also [21]).

It is well-known that the $U(1)$-Higgs model is anomaly-free. Hence, our initial model can be renormalized such that PGI (54) holds true for all values of $m, m_H > 0$. Using Theorem 3.1, we conclude that this model is consistent at all scales.

4 Higgs Mechanism at all Scales to 1-Loop Order

In this section we explain, how one can fulfill the validity of the Higgs mechanism at all scales, i.e. the Eqs. (30), (31), (32), (33), (34), (35), (36), (37), (38), (39) and (40), on 1-loop level.

4.1 The Two Ways to Renormalize

To write the fundamental formula (45) to n-th order, we use the chain rule:

$$Z^{(n)}_{\rho,\mathbf{m}}\big(L(g)^{\otimes n}\big) = \sigma_\rho \circ T_{n\,\mathbf{m}/\rho}\big((\sigma_\rho^{-1}\,L(g))^{\otimes n}\big) - T_{n\,\mathbf{m}}\big(L(g)^{\otimes n}\big) - \sum_{P\in\mathrm{Part}(\{1,\dots,n\}),\, n>|P|>1} T_{|P|\,\mathbf{m}}\big(\otimes_{I\in P} Z^{|I|}_{\rho,\mathbf{m}}(L(g)^{\otimes|I|})\big)\,, \tag{55}$$

where $Z^{(n)}_\rho := Z^{(n)}_\rho(0)$ is the n-th derivative of $Z_\rho(F)$ at $F = 0$ and the two terms with $|P| = n$ and $|P| = 1$, resp., are explicitly written out.

We are now going to investigate the contribution to the r.h.s. of (55) of a primitive divergent diagram Γ, i.e. Γ has singular order[3] $\omega(\Gamma) \geq 0$ and does not contain any subdiagram $\Gamma_1 \subset \Gamma$ with less vertices and with $\omega(\Gamma_1) \geq 0$. For such a diagram, the expression in the second line of (55) vanishes.

Denoting the contribution of Γ to $T_{n\,\mathbf{m}}\big(L(g)^{\otimes n}\big)$ by

$$\int dx_1 \dots dx_n\; t^\Gamma_{\mathbf{m}}(x_1 - x_n, \dots, x_{n-1} - x_n)\, P^\Gamma(x_1, \dots, x_n) \prod_{k=1}^{n} (\kappa g(x_k))^{j_k}$$

(where $P^\Gamma(x_1, \dots, x_n)$ is a, in general non-local, field monomial and the values of $j_1, \dots, j_n \in \{1, 2\}$ depend on Γ), the computation of the contribution of Γ to $Z^{(n)}_{\rho,\mathbf{m}}\big(L(g)^{\otimes n}\big)$ amounts to the computation of

$$\rho^{D^\Gamma}\, t^\Gamma_{\mathbf{m}/\rho}(\rho y) - t^\Gamma_{\mathbf{m}}(y)\,, \tag{56}$$

where $D^\Gamma := \omega(\Gamma) + 4(n-1) \in \mathbb{N}$ and $y := (x_1 - x_n, \dots, x_{n-1} - x_n)$.

For simplicity we assume that $0 \leq \omega(\Gamma) < 2$; this assumption is satisfied for all 1-loop calculations which are done in [5] and whose results are used in this paper. Applying the scaling and mass expansion ("sm-expansion") [4], we then know that $t^\Gamma_{\mathbf{m}}$ is of the form

$$t^\Gamma_{\mathbf{m}}(y) = t^\Gamma(y) + r^\Gamma_{\mathbf{m}}(y)\,, \quad r^\Gamma_{\mathbf{m}} = \mathcal{O}(\mathbf{m}^2)\,, \quad \omega(r^\Gamma_{\mathbf{m}}) < 0\,, \tag{57}$$

[3] For $t \in \mathcal{D}'(\mathbb{R}^l)$ or $t \in \mathcal{D}'(\mathbb{R}^l\backslash\{0\})$, the singular order is defined as $\omega(t) := \mathrm{sd}(t) - l$, where $\mathrm{sd}(t)$ is Steinmann's scaling degree of t, which measures the UV-behaviour of t [20]. In the Epstein-Glaser framework, renormalization is the extension of a distribution $t^\circ \in \mathcal{D}'(\mathbb{R}^l \setminus \{0\})$ to a distribution $t \in \mathcal{D}'(\mathbb{R}^l)$, with the condition that $\mathrm{sd}(t) = \mathrm{sd}(t^\circ)$. In the case $\mathrm{sd}(t^\circ) < l$, the extension is unique, due to the scaling degree requirement, and obtained by "direct extension", see [2, Theorem 5.2], [6, Appendix B] and [11, Theorem 4.1].

where $t^\Gamma := t^\Gamma_{\mathbf{m}=\mathbf{0}}(y)$ (i.e. all Feynman propagators are replaced by their massless version). The remainder scales homogeneously, $\rho^{D^\Gamma} r^\Gamma_{\mathbf{m}/\rho}(\rho y) = r^\Gamma_{\mathbf{m}}(y)$, because it can be renormalized by direct extension (see Footnote 3).

To investigate $\rho^{D^\Gamma} t^\Gamma(\rho y) - t^\Gamma(y)$, we omit the upper index Γ and use the notations $\omega := \omega(\Gamma)$, $l := (n-1)$ and $Y_j := y_j^2 - i_0$. We start with the unrenormalized version $t^\circ \in \mathcal{D}'(\mathbb{R}^{4l} \setminus \{0\})$ of $t := t^\Gamma$, which scales homogeneously:

$$\rho^{\omega+4l}\, t^\circ(\rho y) = t^\circ(y)\ . \tag{58}$$

We work with an analytic regularization [14]:

$$t^{\zeta\circ}(y) := t^\circ(y)\,(M^{2l} Y_1 \dots Y_l)^\zeta\ , \tag{59}$$

where $\zeta \in \mathbb{C} \setminus \{0\}$ with $|\zeta|$ sufficiently small, and $M > 0$ is a renormalization mass scale. $t^{\zeta\circ}$ scales also homogeneously – by the regularization we gain that the degree (of the scaling) is $(\omega+4l-2l\zeta)$, which is not an integer. Therefore, the homogeneous extension $t^\zeta \in \mathcal{D}'(\mathbb{R}^{4l})$ is unique and can explicitly be written down by differential renormalization [11, Sect. IV.D].

Using minimal subtraction for the limit $\zeta \to 0$ we obtain an admissible extension $t^M \in \mathcal{D}'(\mathbb{R}^{4l})$ of t° [11, Corollary 4.4]:

$$\begin{aligned} t^M(y) = \frac{(-1)^\omega}{\omega!} \sum_{r_1 \dots r_{\omega+1}} \partial_{y_{r_{\omega+1}}} \dots \partial_{y_{r_1}} \Big[\frac{1}{2l} \Big(\overline{y_{r_1} \dots y_{r_{\omega+1}}\, t^\circ(y)\, \log(M^{2l} Y_1 \dots Y_l)} \Big) \\ + \Big(\sum_{j=1}^{\omega} \frac{1}{j}\Big) \Big(\overline{y_{r_1} \dots y_{r_{\omega+1}}\, t^\circ(y)} \Big) \Big]\ , \end{aligned} \tag{60}$$

where $\sum_r \partial_{y_r}(y_r \dots) := \sum_r \partial^{y_r}_\mu (y_r^\mu \dots)$ and the overline denotes the direct extension. By means of (57) we obtain the corresponding distribution of the massive model: $t^M_{\mathbf{m}} := t^M(y) + r_{\mathbf{m}}$. In the following we use that

$$\frac{(-1)^\omega}{\omega!} \sum_{r_1 \dots r_{\omega+1}} \partial_{y_{r_{\omega+1}}} \dots \partial_{y_{r_1}} \Big(\overline{y_{r_1} \dots y_{r_{\omega+1}}\, t^\circ(y)} \Big) = \sum_{|a|=\omega} C_a\, \partial^a \delta(y)$$

for some M-independent numbers $C_a \in \mathbb{C}$, as explained after formula (104) in [11].

Whether the expression (56) vanishes depends on the following choice:

(A) if we choose for M a fixed mass scale, which is independent of m, m_H, homogeneous scaling is broken:

$$\begin{aligned} \rho^{\omega+4l}\, t^M_{\mathbf{m}/\rho}(\rho y) - t^M_{\mathbf{m}}(y) &= \rho^{\omega+4l}\, t^M(\rho y) - t^M(y) \\ &= \log\rho \sum_{|a|=\omega} C_a\, \partial^a \delta(y)\ . \end{aligned} \tag{61}$$

The breaking term is unique, i.e. independent of M; therefore, we may admit different values of M for different diagrams, however, all M's must be independent of m, m_H.

(B) In contrast, choosing M such that it is subject to our scaling transformation, i.e. $M := \alpha_1 m + \alpha_2 m_H$ where $(\alpha_1, \alpha_2) \in (\mathbb{R}^2 \setminus \{(0,0)\})$ may be functions of $\frac{m}{m_H}$, the diagram Γ does not contribute to the RG-flow:

$$\rho^{\omega+4l}\, t^{M/\rho}_{\mathbf{m}/\rho}(\rho y) - t^{M}_{\mathbf{m}}(y) = \rho^{\omega+4l}\, t^{M/\rho}(\rho y) - t^{M}(y) = 0\,. \tag{62}$$

Remark 4.1 The requirement that the initial $U(1)$-Higgs model fulfills PGI, is neither in conflict with method (A) nor with method (B), for the following reason: we require PGI only for the initial model. Now, working at one fixed scale, the renormalization constant M appearing in (60) may have any value $M > 0$ for both methods (A) and (B) and, hence, one may choose it such that PGI is satisfied. These methods only prescribe how M behaves under a scaling transformation: using (A) it remains unchanged, using (B) it is also scaled: $M \mapsto \rho^{-1} M$.

4.2 Equality of Certain Coefficients to 1-Loop Order

We explain the basic idea in terms of the two diagrams

$$t^{\circ}_{1\,\mathbf{m}}(y) := \omega_0\Big(T_2(A^\mu\varphi(x_1) \otimes A^\nu\varphi(x_2))\Big) = -\hbar^2 g^{\mu\nu}\, \Delta^F_m(y)\, \Delta^F_{m_H}(y)\,,$$
$$t^{\circ}_{2\,\mathbf{m}}(y) := \omega_0\Big(T_2(A^\mu B(x_1) \otimes A^\nu B(x_2))\Big) = -\hbar^2 g^{\mu\nu}\, (\Delta^F_m(y))^2\,,$$

$t^{\circ}_{1\,\mathbf{m}}, t^{\circ}_{2\,\mathbf{m}} \in \mathcal{D}'(\mathbb{R}^4 \setminus \{0\})$, where ω_0 denotes the vacuum state and $y := x_1 - x_2$. These diagrams are related by the exchange of an inner φ-line with an inner B-line. The essential point is that in the sm-expansion of these two distributions,

$$t^{\circ}_{j\,\mathbf{m}}(y) = t^{\circ}_{j}(y) + r^{\circ}_{j\,\mathbf{m}}(y)\,, \quad r^{\circ}_{j\,\mathbf{m}} = \mathcal{O}(\mathbf{m}^2)\,, \quad \omega(r^{\circ}_{j\,\mathbf{m}}) < 0\,, \quad j = 1, 2\,, \tag{63}$$

the first term (which is the corresponding massless distribution) is the same: $t^{\circ}_1(y) = (D^F(y))^2 = t^{\circ}_2(y)$.

Renormalization is done by extending each term on the r.h.s. of (63) individually and by composing these extensions: $t_{j\,\mathbf{m}} := t_j + r_{j\,\mathbf{m}} \in \mathcal{D}'(\mathbb{R}^4)$. For the remainders $r^{\circ}_{j\,\mathbf{m}}$ the direct extension applies (see Footnote 3), which maintains homogeneous scaling: $\rho^4\, r_{j\,\mathbf{m}/\rho}(\rho y) = r_{j\,\mathbf{m}}(y)$. We conclude: if we renormalize t°_1 and t°_2 both by method (A) or both by method (B), we obtain

$$\begin{aligned}\rho^4\, t_{1\,\mathbf{m}/\rho}(\rho y) - t_{1\,\mathbf{m}}(y) &= \rho^4\, t_1(\rho y) - t_1(y) \\ &= \rho^4\, t_2(\rho y) - t_2(y) = \rho^4\, t_{2\,\mathbf{m}/\rho}(\rho y) - t_{2\,\mathbf{m}}(y)\,.\end{aligned}$$

We point out that different renormalization mass scales M for t_1 and t_2 are admitted, only their behaviour under the scaling transformation must be the same. Therefore, this renormalization prescription is compatible with PGI of the initial $U(1)$-Higgs model.

Renormalizing certain Feynman diagrams, which go over into each other by exchanging $B \leftrightarrow \varphi$ for some lines, by the same method (in this sense) – also triangle and square diagrams with derivatives are concerned – we obtain that some of the coefficients e_ρ agree to 1-loop order:

$$c^{(1)}_{0\rho} = b^{(1)}_{0\rho}\ ,\ \ l^{(1)}_{1\rho} = l^{(1)}_{2\rho}\ ,\ \ l^{(1)}_{3\rho} = l^{(1)}_{4\rho}\ ,\ \ l^{(1)}_{5\rho} = l^{(1)}_{6\rho}\ ,\ \ l^{(1)}_{7\rho} = l^{(1)}_{8\rho} = l^{(1)}_{9\rho}\ , \tag{64}$$

for details see [5]. With that the Eqs. (31), (33), (35) and (37)–(38) are fulfilled.

In addition, the condition

$$l^{(1)}_{11\rho} = 0\ , \tag{65}$$

which is (39) to 1-loop order, can be derived from the stability of PC under the RG-flow, by selecting from (44) the local terms which are $\sim A^2\, A\partial u$ and by using results of Appendix A in [8].

4.3 Changing the Running Interaction by Finite Renormalization

On our way to fulfill the Eqs. (30), (31), (32), (33), (34), (35), (36), (37), (38), (39) and (40) on 1-loop level, we may use that the following finite renormalizations are admitted by the axioms of causal perturbation theory [4, 6, 12] and that they preserve PGI of the initial model: to $T_2\big(L_1(x_1) \otimes L_1(x_2)\big)$ we may add

$$\begin{aligned}\hbar^2 \Big(&\alpha_1\, (\partial\varphi)^2(x_1) + \alpha_2\, m_H^2\, \varphi^2(x_1) + \alpha_3\, F^2(x_1) + \alpha_4\, (\partial A + mB)^2 \\ &+ \alpha_5 \left(-m^2\, B^2(x_1) + (\partial B)^2(x_1)\right) + \alpha_6 \big(m^2\, A^2(x_1) - (\partial A)^2(x_1)\big) \\ &+ \alpha_7\, m^2 \left(-2\,\tilde{u}u(x_1) + A^2(x_1) - B^2(x_1)\right)\Big)\, \delta(x_1 - x_2)\, \log \tfrac{m}{M}\ ,\end{aligned} \tag{66}$$

where $\alpha_1, \ldots, \alpha_7 \in \mathbb{C}$ are arbitrary.

These finite renormalizations modify the 1-loop coefficients $e^{(1)}_\rho$ appearing in $z_\rho(L)$ (17) as follows:

$$a^{(1)}_{0\rho} \mapsto a^{(1)}_{0\rho} + 2i\,\alpha_3\, \log \rho\ , \tag{67}$$

$$a^{(1)}_{1\rho} \mapsto a^{(1)}_{1\rho} - i\,(\alpha_6 + \alpha_7)\, \log \rho\ , \tag{68}$$

$$a^{(1)}_{2\rho} \mapsto a^{(1)}_{2\rho} + i\,(\alpha_4 - \alpha_6)\,\log\rho\,, \tag{69}$$

$$b^{(1)}_{0\rho} \mapsto b^{(1)}_{0\rho} - i\,\alpha_5\,\log\rho\,, \tag{70}$$

$$b^{(1)}_{1\rho} \mapsto b^{(1)}_{1\rho} + i\,(\alpha_4 - \alpha_5 - \alpha_7)\,\log\rho\,, \tag{71}$$

$$b^{(1)}_{2\rho} \mapsto b^{(1)}_{2\rho} + i\,\alpha_4\,\log\rho\,, \tag{72}$$

$$c^{(1)}_{0\rho} \mapsto c^{(1)}_{0\rho} - i\,\alpha_1\,\log\rho\,, \tag{73}$$

$$c^{(1)}_{1\rho} \mapsto c^{(1)}_{1\rho} + i\,\alpha_2\,\log\rho\,, \tag{74}$$

$$c^{(1)}_{2\rho} \mapsto c^{(1)}_{2\rho} - i\,\alpha_7\,\log\rho\,, \tag{75}$$

the other coefficients remain unchanged.

We did not find any further finite renormalizations, which fulfill, besides the already mentioned conditions, the following requirements:

– that they do not add "by hand" novel kind of terms to $(z_\rho(L) - L)$ (see (17)) as e.g. terms $\sim \partial\tilde{u}\partial u$ or $\sim m\,\tilde{u}u\varphi$, and
– that the Eqs. (64) are preserved.

See [5] for details.

4.4 How to Fulfill the Higgs Mechanism at all Scales

There are two necessary conditions for the Higgs mechanism at all scales, which are crucial, since they cannot be fulfilled by finite renormalizations.

Verification of the first crucial necessary condition The condition (41) reads to 1-loop level

$$l^{(1)}_{7\rho} - l^{(1)}_{3\rho} = l^{(1)}_{5\rho} - l^{(1)}_{0\rho}\,. \tag{76}$$

Since the admissible finite renormalizations (66) do not modify the coefficients $l^{(1)}_{j\rho}$, there is no possibility to fulfill (76) in this way. However, computing explicitly the relevant coefficients $l^{(1)}_{j\rho}$ by using the renormalization method (A) for all contributing terms, we find that (76) holds indeed true. This computation, which is given in [5], involves cancellations of square- and triangle-diagrams – this shows that (76) is of a deeper kind than the equalities derived in Sect. 4.2.

The identity (76) holds also if certain classes of corresponding diagrams are renormalized by method (B).

How to fulfill the second crucial necessary condition The condition (40) reads to 1-loop order

$$b^{(1)}_{2\rho} = \tfrac{1}{2}\big(a^{(1)}_{2\rho} + b^{(1)}_{1\rho} - a^{(1)}_{1\rho} - b^{(1)}_{0\rho}\big)\,. \tag{77}$$

Performing the finite renormalizations (66), i.e. inserting (67), (68), (69), (70), (71), (72), (73), (74) and (75) into (77), we find that all α_j drop out – that is, the condition (77) cannot be fulfilled by means of these finite renormalizations.

Computing the explicit values for the coefficients $a^{(1)}_{j\rho}$, $b^{(1)}_{j\rho}$ by using method (A) (see [5]), we find that (77) does not hold. Hence, using method (A) throughout, we have $\lambda_{12\rho} \neq 0$, i.e. the geometrical interpretation (27) is violated by terms $\sim A\partial B$.

However, we can fulfill the condition (77) by switching the method from (A) to (B) for all diagrams contributing to $b^{(1)}_{1\rho}$ and a part of the diagrams contributing to $a^{(1)}_{1\rho}$ [5]. (This switch concerns also all diagrams contributing to $a^{(1)}_{0\rho}$, hence we obtain $a^{(1)}_{0\rho} = 0$.)

A family of solutions of the Higgs mechanism at all scales The conditions (30), (31), (32), (33), (34), (35), (36), (37), (38), (39) and (40) can be solved to 1-loop order as follows: initially we renormalize all diagrams by using method (A), except for the diagrams just mentioned, for which we use method (B) to fulfill the second crucial necessary condition (77). Then we take into account the possibility to modify the coefficients $e^{(1)}_\rho$ by finite renormalizations (67), (68), (69), (70), (71), (72), (73), (74) and (75). This procedure yields the following family of solutions:

$$\begin{aligned}
&a^{(1)}_{0\rho} = 2\beta_1\, L_\rho\,, \quad a^{(1)}_{1\rho} = -4\, L_\rho\,, \quad a^{(1)}_{2\rho} = (\beta_2 - \beta_3)\, L_\rho\,,\\
&b^{(1)}_{0\rho} = c^{(1)}_{0\rho} = (2 + 2l_1)\, L_\rho\,, \quad b^{(1)}_{1\rho} = (4 + 2l_1 + \beta_2 + \beta_3)\, L_\rho\,,\\
&b^{(1)}_{2\rho} = (3 + \beta_2)\, L_\rho\,, \quad c^{(1)}_{1\rho} = -\Big(6\frac{m^2}{m_H^2} + 5\frac{m_H^2}{m^2}\Big) L_\rho\,, \quad c^{(1)}_{2\rho} = (-1 + \beta_3)\, L_\rho\,,\\
&l^{(1)}_{0\rho} = -3\, L_\rho\,, \quad l^{(1)}_{1\rho} = l^{(1)}_{2\rho} =: l_1\, L_\rho\,, \quad l^{(1)}_{3\rho} = l^{(1)}_{4\rho} = \Big(1 - 6\frac{m^2}{m_H^2} - 5\frac{m_H^2}{m^2}\Big) L_\rho\,,\\
&l^{(1)}_{5\rho} = l^{(1)}_{6\rho} = -2\, L_\rho\,, \quad l^{(1)}_{7\rho} = l^{(1)}_{8\rho} = l^{(1)}_{9\rho} = \Big(2 - 6\frac{m^2}{m_H^2} - 5\frac{m_H^2}{m^2}\Big) L_\rho
\end{aligned} \tag{78}$$

and $l^{(1)}_{11\rho} = 0$, where $L_\rho := \frac{1}{8\pi^2}\log\rho$, the number l_1 is obtained on computing $l^{(1)}_{1\rho} =: l_1\, L_\rho$ by method (A), and $\beta_1 := i8\pi^2\alpha_3$, $\beta_2 := i8\pi^2\alpha_4$, $\beta_3 := i8\pi^2\alpha_6 = -i8\pi^2\alpha_7 \in \mathbb{C}$ are parameters with arbitrary values.

The family (78) is by far not the general solution of the conditions (30), (31), (32), (33), (34), (35), (36), (37), (38), (39) and (40); in particular, there is the

trivial solution $z_\rho(L) = \frac{1}{\hbar}(L + \mathcal{O}(\hbar^2))$ (i.e. $e_\rho^{(1)} = 0\ \forall e$), which is obtained by renormalizing all 1-loop-diagrams by method (B).

To 1-loop order one can even find a non-trivial solution of the clearly stronger property of BRST-invariance of $(L_0 + z_\rho(L))$; but this requires a very specific combination of the methods (A) and (B) for the various 1-loop diagrams and suitable finite renormalizations. Hence, in general, $s(L_0 + z_\rho(L))$ is *not* $\simeq 0$, and also $s_0 L_0$ is *not* $\simeq 0$; in particular these two statements hold for the family (78) – see [5].

4.5 *Frequently used Renormalization Schemes*

In conventional momentum space renormalization a frequently used renormalization scheme is dimensional regularization with minimal subtraction, which preserves BRST-invariance generically. Applied to the 1-loop diagrams of our initial model, this property implies that the resulting time-ordered products fulfill PGI.[4] Dimensional regularization needs a mass scale $M > 0$; which remains in the formulas when removing the regularization by using minimal subtraction, and plays the role of the renormalization mass scale. Usually M is chosen according to method (A); and the minimal subtraction prescription forbids to perform any finite renormalization. Therefore, using this prescription, the Higgs mechanism is not applicable at an arbitrary scale, because the second crucial necessary condition (77) is violated. Relaxing this prescription by admitting the finite PGI-preserving renormalizations (67), (68), (69), (70), (71), (72), (73), (74) and (75), the violation of (77) cannot be removed.

Another state independent renormalization scheme is the central solution of Epstein and Glaser [12]. (For 1-loop diagrams this scheme corresponds to BPHZ-subtraction at $p = 0$.) Since the subtraction point $p = 0$ is scaling invariant, the central solution maintains homogeneous scaling (w.r.t. $(x, \mathbf{m}) \to (\rho x, \mathbf{m}/\rho)$; cf. [4, Sec. 2.3]); hence, the pertinent RG-flow is trivial.

In the conventional literature one meets also state dependent renormalization conditions: e.g. in the adiabatic limit the vacuum expectation values of certain time-ordered products must agree with the "experimentally" known values for the masses of stable particles in the vacuum, and analogous conditions for parameters of certain vacuum correlation functions. Since "experimental" results are not subject to our scaling transformation, a lot of diagrams are renormalized by method (A), if we use such a scheme. To 1-loop level, the validity of the Higgs mechanism at all scales amounts then mainly to the question: is it nevertheless possible to fulfill the second

[4] We are not aware of a proof of this statement, but it is very plausible. A corresponding statement for higher loop diagrams involves a partial adiabatic limit, because such diagrams contain inner vertices, which are integrated out with $g(x) = 1$ in conventional momentum space renormalization – but PGI is formulated *before* the adiabatic limit $g \to 1$ is taken.

crucial necessary condition (77), which requires to renormalize certain diagrams by method (B)?

5 Summary and Conclusions

In the Epstein-Glaser framework the obvious way to define the RG-flow is to use the Main Theorem in the adiabatic limit [3, 6, 15, 18]: the effect of a scaling transformation (scaling with $\rho > 0$) can equivalently be expressed by a renormalization of the interaction: $L \mapsto z_\rho(L)$. The so defined RG-flow $\rho \mapsto z_\rho(L)$ depends on the choice of the renormalization mass scale(s) $M > 0$ for the various UV-divergent Feynman diagrams: if M is subject to our scaling transformation (method (B)) – e.g. the mass of one of the basic fields – the pertinent diagram does not contribute to the RG-flow. In contrast, if M is a fixed mass scale (method (A)), the corresponding diagram yields a unique (i.e. M-independent), non-vanishing contribution.

Performing the renormalization of the wave functions, masses, gauge-fixing parameter and coupling parameters, we obtain a description of the scaled model $L_0 + z_\rho(L)$ (L_0 denotes the free Lagrangian) by a new Lagrangian $L_0^\rho + L^\rho$, which has essentially the same form as the original one, $L_0 + L$; but the basic fields and the parameters are ρ-dependent. The title of this paper can be reformulated as follows: is the new Lagrangian $L_0^\rho + L^\rho$ derivable by the Higgs mechanism for all $\rho > 0$?

We have investigated this question for the $U(1)$-Higgs model to 1-loop order. We only admit renormalizations of the initial model which fulfill a suitable form of BRST-invariance of the time-ordered products – we work with PGI (54). The answer depends not only on the choice of the renormalization method ((A) or (B)) for the various 1-loop Feynman diagrams; the RG-flow can also be modified by finite, PGI-preserving renormalizations (66) of the initial model. Using this non-uniqueness, we have shown that one can achieve that the Higgs mechanism is possible at all scales; one can even fulfill the much stronger condition of BRST-invariance of $L_0 + z_\rho(L)$. But this requires a quite (Higgs mechanism) or very (BRST-invariance) specific prescription for the choice of the renormalization method ((A) or (B)) for the various Feynman diagrams, and for the finite renormalizations. If one uses always method (A) – minimal subtraction is of this kind – the geometrical interpretation is violated by terms $\sim A\partial B$; weakening this prescription by admitting finite PGI-preserving renormalizations, these $A\partial B$-terms cannot be removed.

If one accepts the Higgs mechanism as a fundamental principle explaining the origin of mass at all scales (although it is not understood in a pure QFT framework), our results exclude quite a lot of renormalization schemes, in particular minimal subtraction.

On the other hand we give a model-independent proof, which uses rather weak assumptions, that the RG-flow is compatible with a weak form of BRST-invariance of the time-ordered products, namely PC (Theorem 3.1). However, in [5] it is shown that the somewhat stronger property of PGI gets lost under the RG-flow in

general, and in particular if one uses a renormalization prescription corresponding to minimal subtraction.

Acknowledgements During working at this paper the author was mainly at the Max Planck Institute for Mathematics in the Sciences, Leipzig; he thanks Eberhard Zeidler for the invitations to Leipzig and for valuable discussions. In addition, the author profitted from invitations to give a talk about the topic of this paper at the workshop "Algebraic Quantum Field Theory: Its status and its future" at the Erwin Schröder Institute in Vienna (19.-23.05.2014) and at the conference "Quantum Mathematical Physics" in Regensburg (29.09.-02.10.2014). The author thanks also the Vicerrectoría de Investigación of the Universidad de Costa Rica for financial support. The question in the title of this paper was found during innumerable discussions with Jürgen Tolksdorf about his geometrical derivation of a value for the Higgs mass. The author also profitted a lot from stimulating discussions with Klaus Fredenhagen, José M. Gracia-Bondía, Bert Schroer, Günter Scharf, Klaus Sibold and Joseph C. Várilly.

References

1. A. Aste, M. Dütsch, G. Scharf, Perturbative gauge invariance: the electroweak theory II. Ann. Phys. (Leipzig) **8**(5), 389–404 (1999)
2. R. Brunetti, K. Fredenhagen, Microlocal analysis and interacting quantum field theories: renormalization on physical backgrounds. Commun. Math. Phys. **208**, 623–661 (2000)
3. R. Brunetti, M. Dütsch, K. Fredenhagen, Perturbative algebraic quantum field theory and the renormalization groups. Adv. Theor. Math. Phys. **13**, 1541–1599 (2009)
4. M. Dütsch, The scaling and mass expansion. Ann. Henri Poincaré **16**(1), 163–188 (2015). doi:10.1007/s00023-014-0324-6
5. M. Dütsch, Massive vector bosons: is the geometrical interpretation as a spontaneously broken gauge theory possible at all scales?. arXiv:1501.02599
6. M. Dütsch, K. Fredenhagen, Causal perturbation theory in terms of retarded products, and a proof of the Action Ward Identity. Rev. Math. Phys. **16**, 1291–1348 (2004)
7. M. Dütsch, G. Scharf, Perturbative gauge invariance: the electroweak theory. Ann. Phys. (Leipzig) **8**(5), 359–387 (1999)
8. M. Dütsch, B. Schroer, Massive vector mesons and gauge theory. J. Phys. A **33**(23), 4317–4356 (2000)
9. M. Dütsch, T. Hurth, F. Krahe, G. Scharf, Causal construction of Yang-Mills theories II. Il Nuovo Cimento A **107**, 375–406 (1994)
10. M. Dütsch, J.M. Gracia-Bondía, F. Scheck, J.C. Várilly, Quantum gauge models without (classical) Higgs mechanism. Eur. Phys. J. C. **69.3**, 599–622 (2010)
11. M. Dütsch, K. Fredenhagen, K.J. Keller, K. Rejzner, Dimensional regularization in position space, and a forest formula for Epstein-Glaser renormalization. J. Math. Phys. **55**, 122303 (2014). doi:10.1063/1.4902380
12. H. Epstein, V. Glaser, The role of locality in perturbation theory. Ann. Inst. Henri Poincaré **19A**, 211–295 (1973)
13. H. Epstein, V. Glaser, Adiabatic limit in perturbation theory, in *Renormalization Theory,* ed. by G. Velo, A.S. Weightman (D. Riedel Publishing Company, Dordrecht, 1976), pp. 193–254
14. S. Hollands, Renormalized quantum Yang-Mills fields in curved spacetime. Rev. Math. Phys. **20**, 1033–1172 (2008)
15. S. Hollands, R.M. Wald, On the renormalization group in curved spacetime. Commun. Math. Phys. **237**, 123–160 (2003)
16. S. Hollands, R.M. Wald, On the renormalization group in curved spacetime. Rev. Math. Phys. **17**, 227–312 (2005)

17. T. Kugo, I. Ojima, Local covariant operator formalism of non-abelian gauge theories and quark confinement problem. Suppl. Progr. Theor. Phys. **66**(6), 1 (1979)
18. G. Popineau, R. Stora, *A Pedagogical Remark on the Main Theorem of Perturbative Renormalization Theory* (LAPP–TH, Lyon, 1982)
19. G. Scharf, *Quantum Gauge Theories: A True Gost Story* (Wiley, New York, 2001)
20. O. Steinmann, *Perturbation Expansions in Axiomatic Field Theory*. Lecture Notes in Physics, vol. 11 (Springer, Berlin, 1971)
21. R. Stora, Local gauge groups in quantum field theory: Perturbative gauge theories. Talk given at the workshop 'Local Quantum Physics' at the Erwin-Schrödinger-Institut, Vienna 1997

Hadamard States From Null Infinity

Claudio Dappiaggi

Contents

Abstract Free field theories on a four dimensional, globally hyperbolic spacetime, whose dynamics is ruled by a Green hyperbolic partial differential operator, can be quantized following the algebraic approach. It consists of a two-step procedure: In the first part, one identifies the observables of the underlying physical system collecting them in a $*$-algebra which encodes their relational and structural properties. In the second step, one must identify a quantum state, that is a positive, normalized linear functional on the $*$-algebra out of which one recovers the interpretation proper of quantum mechanical theories via the so-called Gelfand-Naimark-Segal theorem. In between the plethora of possible states, only few of them are considered physically acceptable and they are all characterized by the so-called Hadamard condition, a constraint on the singular structure of the associated two-point function. The goal of this paper is to outline a construction scheme for these states which can be applied whenever the underlying background possesses a null (conformal) boundary. We discuss in particular the examples of a real, massless conformally coupled scalar field and of linearized gravity on a globally hyperbolic and asymptotically flat spacetime.

C. Dappiaggi (✉)
Dipartimento di Fisica & INFN, Sezione di Pavia, Università degli Studi di Pavia, Via Bassi 6, I-27100 Pavia (PV), Italy
e-mail: claudio.dappiaggi@unipv.it

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_5

Keywords Quantum field theory on curved backgrounds • Algebraic quantum field theory

Mathematics Subject Classification (2010). Primary 81T20; Secondary 81T05

1 Introduction

Quantum field theory on curved backgrounds has witnessed a period of renaissance in the past 20 years. From a physical perspective, cosmology is acquiring an everyday greater relevance, mostly on account of the expected, upcoming plethora of experimental data. The models with which these should be compared are often aimed at the description of the dynamics of the evolution of the early Universe and are mainly based on fields living on homogeneous and isotropic manifolds. In this framework quantum effects are expected to play a key role, for example in shaping the fluctuations of the cosmic microwave background.

Understanding quantum field theory beyond Minkowski spacetime has shifted from a purely academic question to a concrete necessity and, thus, it has been accompanied contemporary by an increasing interest in developing its structural, foundational and mathematical aspects. In this respect a framework appears to claim the lion's share of interest: algebraic quantum field theory. In a few words, this is a mathematically rigorous approach based on two key steps. In the first, one codifies the observables of the physical system under investigation into a $*$-algebra $\mathcal{A}$ which encompasses the information about the dynamics, locality and causality. In the second, instead, one identifies a so-called algebraic state, namely a positive, normalized linear functional $\omega : \mathcal{A} \to \mathbb{C}$. Via the Gelfand-Naimark-Segal (GNS) theorem, one associates to the pair $(\mathcal{A}, \omega)$ a triplet of data which in particular identifies a Hilbert space, as well as both a representation of $\mathcal{A}$ in terms of linear operators thereon and a unit norm, cyclic vector. In other words, one recovers the standard interpretation of quantum mechanical theories. Much has been written about the algebraic approach, especially on curved backgrounds, and we refer an interested reader to the several recent reviews, e.g., [5, 18].

We will be interested, instead, in a more specific problem. For any given algebra $\mathcal{A}$, one can easily construct several algebraic states, but one can hardly call all of them physically relevant. The reasons are manifold and often related to pathological behaviors such as for example the occurrence of divergences in the quantum fluctuations of observables or the impossibility of constructing Wick polynomials, which are the basis to deal with interactions at a perturbative level. Especially for free field theories on globally hyperbolic spacetimes this problem has been thoroughly discussed since the seventies and, by now, it is almost unanimously accepted that a state, to be called physical, must be of *Hadamard form*. Originally it was a condition on the form in each geodesically convex neighborhood of the manifold of the integral kernel of the two-point function. Verifying it in concrete

cases is rather complicated if not outright impossible and, for this reason, for many years only few examples of Hadamard states were known, e.g., the Poincaré vacuum on Minkowski spacetime and the Bunch-Davies state for a scalar field on de Sitter spacetime. Although generic existence results were known via deformation techniques [20], a cornerstone in our understanding of Hadamard states came from the papers of Radzikowski [31, 32]. He showed that the Hadamard condition is fully equivalent to assigning a precise form to the wavefront set of the bi-distribution associated to the two-point correlation function of a quasi-free/Gaussian state. Despite the necessity of using microlocal analysis, controlling explicitly the wavefront set turns out to be much easier in concrete scenarios and, hence, starting from [31, 32], many construction schemes for Hadamard states were devised. In this paper, we review a particular one which originates from a possible transposition to the algebraic framework of the often mentioned holographic principle. Called also bulk-to-boundary correspondence, this constructive scheme was first discussed in [11] and it is devised to work for free field theories on four dimensional globally hyperbolic spacetimes possessing a null (conformal) boundary. The main idea is based on the observation that the generators of the observables of a free field theory are in correspondence with smooth and spacelike compact solutions of the underlying equations of motion. On account of the properties of the (unique) Green operators associated to the underlying dynamics, each of these solutions propagates to the null boundary identifying thereon a smooth function. Hence, by constructing a suitable $*$-algebra of functions on the null boundary, one can put the algebra of observables of a free field theory in correspondence with a $*$-subalgebra of the boundary one. More importantly this entails that each algebraic state on the boundary identifies a counterpart for the free field theory living on the bulk spacetime. The net advantage of this procedure is twofold: On the one hand, the boundary usually possesses an infinite dimensional symmetry group, which, exactly as the Poincaré group in Minkowski spacetime, allows to identify a distinguished state thereon. On the other hand, the theorem of propagation of singularities in combination with a control of the wavefront set of the Green operators allows us to prove that such distinguished, boundary state induces a bulk counterpart of Hadamard form.

Up to now this procedure has been applied successfully in several different contexts and for different theories ranging from scalar fields on cosmological spacetimes [12, 13] and on black hole spacetimes [9, 13], to Dirac fields on cosmological and asymptotically flat spacetimes [15], to free electromagnetism [10]. It is noteworthy that this procedure allows also for the identification of local ground states [16] and it is suitable to be translated in the language of pseudodifferential calculus, as shown recently in these interesting papers [21–23].

Since we cannot go into the details of all these results, we decided to focus our attention on two special but instructive applications of the bulk-to-boundary correspondence. The first discusses the procedure for a real, massless and conformally coupled scalar field on asymptotically flat spacetimes [11]. The second instead aims at reviewing the most recent application of this construction and at showing the

additional complications arising for linear gauge theories, namely we shall discuss linearized gravity following [6].

The paper is organized as follows: In Sect. 2, we outline the classical dynamics of a real scalar field and the construction of the algebra of fields. In Sect. 2.1, first we introduce the class of asymptotically flat and globally hyperbolic, four dimensional spacetimes and, subsequently, we discuss the bulk-to-boundary correspondence and particularly the construction of a Hadamard state for a massless, conformally coupled scalar field. In Sect. 3, we focus our attention on linearized gravity and we show how to construct an algebra of fields while dealing with gauge freedom. To conclude, in Sect. 3.1, we repeat briefly the construction of Hadamard states starting from future null infinity, focusing mainly on the additional problems brought by gauge invariance. On account of the lack of space, we plan to avoid giving detailed proofs of all mathematical statements, referring each time instead to the relevant literature.

2 Scalar Field Theory

In this section, we shall outline the quantization within the algebraic framework of the simplest example of field theory. First of all, we need to specify the class of backgrounds which we consider as admissible and which, henceforth, are referred to as spacetimes. We allow only four dimensional, connected, smooth manifolds M endowed with a smooth Lorentzian metric g of signature $(-,+,+,+)$. Furthermore, we require (M,g) to be globally hyperbolic, that is M possesses a Cauchy surface Σ, a closed achronal subset of M whose domain of dependence coincides with the whole spacetime – for more details, refer to [34, Ch. 8]. The existence of a Cauchy surface leads to several noteworthy consequences. In between them, we stress that the property of being globally hyperbolic entails in particular that M is isometric to the Cartesian product $\mathbb{R}\times\Sigma$ and thereon there exists a coordinate system such that the line element reads

$$ds^2 = -\beta dt^2 + h_t.$$

Here $t:\mathbb{R}\times\Sigma\to\mathbb{R}$ is the projection on the first factor, while β is a smooth and strictly positive scalar function on $\mathbb{R}\times\Sigma$. Furthermore, for all values of t, $\{t\}\times\Sigma$ is a 3-dimensional smooth, spacelike, Cauchy surface in M and $t\mapsto h_t$ is a one-parameter family of smooth Riemannian metrics – see [4, 8] and references therein.

Besides a globally hyperbolic spacetime (M,g), we consider a real scalar field $\phi:M\to\mathbb{R}$ whose dynamics is ruled by the Klein-Gordon equation

$$P\phi = \left(\Box - m^2 - \xi R\right)\phi = 0, \tag{1}$$

where $m\geq 0$ is the mass, R is scalar curvature built out of g, while $\xi\in\mathbb{R}$ is a coupling constant. While all values of ξ are admissible and, from a structural point

of view, they are all equivalent, two cases are often considered in the literature: $\xi = 0$, also known as *minimal coupling* or $\xi = \frac{1}{6}$, the *conformal coupling*. In this paper, we will be interested mainly in this last option, moreover, with a vanishing mass. Regardless of the value of m and ξ, the operator P is a special case of a Green hyperbolic partial differential operator – refer to [2]. Hence, the smooth solutions of (1) can be constructed in terms of a Cauchy problem, for which smooth initial data are assigned on any but fixed Cauchy surface $\{t\} \times \Sigma$. Yet, this approach breaks manifestly covariance and, especially from the perspective of the algebraic quantization scheme, it is more appropriate to adopt a different approach, namely that of Green functions. To this end, we introduce a notable class of functions:

Definition 2.1 We call $C^\infty_{tc}(M)$ the collection of all *timelike compact* functions, that is $f \in C^\infty_{tc}(M)$ if f is a smooth function such that, for all $p \in M$, $\mathrm{supp}(f) \cap J^\pm(p)$ is either empty or compact. Here $J^\pm(p)$ stands for the causal future (+) and past (-) of p.

Following [2, 33] and generalizing slightly the content of [3, 4],

Definition 2.2 We call *retarded* (+) and *advanced* (−) *Green operators* associated to the Klein-Gordon operator P, two linear maps $E^\pm : C^\infty_{tc}(M) \to C^\infty(M)$ such that, for every $f \in C^\infty_{tc}(M)$,

$$\left(P \circ E^\pm\right)(f) = f = \left(E^\pm \circ P\right)(f),$$

and $\mathrm{supp}\left(E^\pm(f)\right) \subseteq J^\pm(\mathrm{supp}(f))$. The map $E = E^- - E^+$ is called *causal propagator*.

If we introduce the space of all smooth solutions of (1),

$$\mathcal{S}(M) \doteq \{\phi \in C^\infty(M) \mid P\phi = 0\}, \tag{2}$$

advanced and retarded Green operators can be used to prove two important properties of (1) which we only recollect here:

- There exists an isomorphism of topological vector spaces between $\mathcal{S}(M)$ and $\frac{C^\infty_{tc}(M)}{P[C^\infty_{tc}(M)]}$ which is realized by E. In other words, for every $\phi \in \mathcal{S}(M)$, there exists $[f] \in \frac{C^\infty_{tc}(M)}{P[C^\infty_{tc}(M)]}$ such that $\phi = E(f)$ regardless of the chosen representative in $[f]$.
- Let $\mathcal{S}_{sc}(M) \subset \mathcal{S}(M)$ be the vector subspace of the *spacelike compact*, smooth solutions ϕ to (1), that is $\mathrm{supp}(\phi) \cap (\{t\} \times \Sigma)$ is compact for all values of t. Still via the causal propagator, $\mathcal{S}_{sc}(M)$ is isomorphic to $\frac{C^\infty_0(M)}{P[C^\infty_0(M)]}$, where $C^\infty_0(M)$ is the collection of smooth and compactly supported functions on M. Most notably $\mathcal{S}_{sc}(M)$ is a symplectic space if endowed with the following weakly non-degenerate symplectic form $\sigma : \mathcal{S}_{sc}(M) \times \mathcal{S}_{sc}(M) \to \mathbb{R}$

$$\sigma(\phi, \phi') = E([f], [f']) \doteq \int_M d\mu_g E(f) f', \tag{3}$$

where $d\mu_g$ is the metric-induced volume form, while $[f], [f'] \in \frac{C_0^\infty(M)}{P[C_0^\infty(M)]}$ are such that $\phi^{(\prime)} = E(f^{(\prime)})$.

Having under control the space of all smooth solutions of (1), we can introduce the notion of observable for a real scalar field. Notice that, at this stage, we are still working at a purely classical level. The underlying paradigm is that an observable is nothing but an assignment of a real number to any configuration of a physical system, done in a way which is compatible with the underlying dynamics. At a mathematical level, this heuristic statement can be translated as follows: Let us consider *off-shell/kinematical* configurations, namely all $\phi \in C^\infty(M)$ and, for any $f \in C_0^\infty(M)$, we define the linear functional

$$F_f : C^\infty(M) \to \mathbb{R}, \quad \phi \mapsto F_f(\phi) \doteq \int_M d\mu_g \, \phi(x) f(x). \tag{4}$$

The map F_f plays the role of a classical linear observable for the kinematical configurations of a Klein-Gordon field and, from standard results in functional analysis, we can also infer that the assignment $f \mapsto F_f$ is injective and that the collection of all functionals, built in this way, is separating. This entails that, for every $\phi, \phi' \in C^\infty(M)$, we can find at least one $f \in C_0^\infty(M)$ such that $F_f(\phi) \neq F_f(\phi')$.

In order to codify in this construction the information of the dynamics, it suffices to restrict the kinematical configurations to the dynamically allowed, namely to $\mathcal{S}(M) \subset C^\infty(M)$. In other words we consider now the assignment $f \in C_0^\infty(M) \mapsto F_f : \mathcal{S}(M) \to \mathbb{R}$. While the property of being a separating set is left untouched by the restriction of the configurations allowed, injectivity is no longer valid. As a matter of fact, one can prove that $F_f(\phi) = 0$ for all $\phi \in \mathcal{S}(M)$ if and only if there exists $h \in C_0^\infty(M)$ such that $f = P(h)$. For this reason we identify those linear functionals F_f and $F_{f'}$ on $\mathcal{S}(M)$ such that $f - f' \in P[C_0^\infty(M)]$. To summarize, the space of *linear classical observables* is

$$\mathcal{E}^{obs}(M) \doteq \left\{ F_{[f]} : \mathcal{S}(M) \to \mathbb{R} \;\middle|\; [f] \in \frac{C_0^\infty(M)}{P[C_0^\infty(M)]} \right\}, \tag{5}$$

where $F_{[f]}(\phi) = F_f(\phi)$, the right-hand side being defined in (4). On the one hand, notice that $\mathcal{E}^{obs}(M)$ is isomorphic to the labeling space $\frac{C_0^\infty(M)}{P[C_0^\infty(M)]}$ and, thus, it comes naturally endowed with the symplectic form (3). On the other hand, we remark that the choice of observables is far from being unique. Our guiding principles have been essentially three: We want $\mathcal{E}^{obs}(M)$ to separate all dynamical configurations, to lack any redundant observable and to be a symplectic space. While in the analysis of a real scalar field, our approach might look as an overkill, which ultimately yields already well-known results, we stress that the paradigm that we used is very effective as soon as we deal with gauge theories – see for example [7].

Having under control the dynamics of a real scalar field and having chosen a linear space of classical observables is the starting point of the quantization scheme that we follow. As mentioned in the introduction the algebraic scheme is based on two steps, the first of which consists of regrouping all observables into a suitable $*$-algebra. Starting from (5),

Definition 2.3 We call **algebra of fields** for a real scalar field, whose dynamics is ruled by (1), the quotient $\mathcal{F}(M) = \frac{\mathcal{T}(M)}{\mathcal{I}(M)}$. Here

$$\mathcal{T}(M) \doteq \bigoplus_{n=0}^{\infty} \mathcal{E}^{obs}(M;\mathbb{C})^{\otimes n},$$

is the universal tensor algebra endowed with complex conjugation as $*$-operation, where $\mathcal{E}^{obs}(M;\mathbb{C}) = \mathcal{E}^{obs}(M) \otimes \mathbb{C}$ while $\mathcal{E}^{obs}(M;\mathbb{C})^{\otimes 0} \doteq \mathbb{C}$. $\mathcal{I}(M)$ is the $*$-ideal generated by the *canonical commutation relations* $[f] \otimes [f'] - [f'] \otimes [f] - iE([f],[f'])\,\mathbb{I}$, where $\mathbb{I}$ is the identity in $\mathcal{T}(M)$.

Notice that in the definition we have used implicitly the identification between classical observables and the labeling space $\frac{C_0^\infty(M)}{P[C_0^\infty(M)]}$ while $E([f],[f'])$ is the symplectic form (3). Although much has been written in the literature about $\mathcal{F}(M)$, we want to recall here two of its most important properties, the proof of which can be found for example in [6].

Proposition 2.4 *The algebra of fields $\mathcal{F}(M)$*

1. *is **causal**, that is elements of $\mathcal{F}(M)$ localized in causally disjoint regions commute,*
2. *fulfills the **time-slice axiom**. Let $\mathcal{O} \subset M$ be a globally hyperbolic open neighborhood of a spacelike Cauchy surface Σ, that is $\mathcal{O}$ contains all causal curves for (M, g) whose endpoints lie in $\mathcal{O}$. Let $\mathcal{F}(\mathcal{O})$ be the algebra of fields for a real scalar field in $(\mathcal{O}, g|_{\mathcal{O}})$. Then $\mathcal{F}(\mathcal{O})$ is $*$-isomorphic to $\mathcal{F}(M)$.*

We have completed the first part of the algebraic quantization procedure and, thus, we are left with the second and last one. From a more general point of view, given any unital $*$-algebra $\mathcal{A}$, we call *algebraic state* a positive and normalized linear functional $\omega : \mathcal{A} \to \mathbb{C}$ such that

$$\omega(\mathbb{I}) = 1, \qquad \omega(a^* a) \geq 0, \ \forall\, a \in \mathcal{A},$$

where $\mathbb{I}$ is the unit of $\mathcal{A}$. States are relevant since, in combination with $\mathcal{A}$, they allow for recovering the probabilistic interpretation proper of quantum theories via the celebrated GNS theorem, which we recollect here – see [30, Ch. 14]:

Theorem 2.5 *Let ω be a state on a unital $*$-algebra $\mathcal{A}$. There exists a dense subspace $\mathcal{D}$ of a Hilbert space $(\mathcal{H}, (\cdot,\cdot))$, as well as a representation $\pi : \mathcal{A} \to \mathcal{L}(\mathcal{D})$ and a unit norm, cyclic vector $\Omega \in \mathcal{D}$, such that $\omega(\cdot) = (\Omega, \pi(\cdot)\Omega)$ and $\mathcal{D} = \pi(\mathcal{A})\Omega$. The* GNS triple $(\mathcal{D}, \pi, \Omega)$ *is uniquely determined up to unitary equivalence.*

We are interested especially in the case where the $*$-algebra is $\mathcal{F}(M)$. In this respect, constructing algebraic states is not a difficult operation and several examples are easily available. Yet, in between all of them, most of these states cannot be considered physically acceptable and one of the biggest challenges in the algebraic approach to quantum field theory has been indeed to identify suitable criteria to single out states which yield a good physical behavior. Especially when one cannot exploit Poincaré covariance to construct a (unique) vacuum state, e.g., when the underlying background is curved, the question is of paramount importance. After long debates it is nowadays almost unanimously accepted that the answer consists of requiring that an algebraic state fulfills the so-called *Hadamard condition*.

From a physical perspective it amounts to saying that a state is physically acceptable if all quantum fluctuations of the observables are finite and if its ultraviolet behavior is close to that of the Poincaré vacuum. Furthermore, the class of Hadamard states allows for a local and covariant construction of Wick polynomials, which is a prerequisite for dealing with interactions at a perturbative level [27]. The translation at a mathematical level is the following. As a starting point, we notice that, since $\mathcal{F}(M)$ is the quotient between $\mathcal{T}(M)$ and $\mathcal{I}(M)$, assigning a state $\omega : \mathcal{F}(M) \to \mathbb{C}$ is equivalent to constructing all n-point correlation functions $\omega_n : \left(C_0^\infty(M)\right)^{\otimes n} \to \mathbb{C}$ fulfilling suitable constraints so to ensure positivity and compatibility both with the dynamics and with the canonical commutations relations. In between all states, most notable are the quasi-free/Gaussian ones, which are characterized by the property of being completely determined by the associated two-point function. With a slight abuse of notation, this is tantamount to choosing a suitable $\omega_2 \in \mathcal{D}'(M \times M)$, extending it via the formula:

$$\omega_{2n}(\lambda_1 \otimes \ldots \otimes \lambda_{2n}) = \sum_{\pi_{2n} \in S_{2n}} \prod_{i=1}^{n} \omega_2(\lambda_{\pi_{2n}(2i-1)} \otimes \lambda_{\pi_{2n}(2i)}), \quad \omega_{2n+1} = 0,$$

where $n \in \mathbb{N}$. Here S_{2n} stands for the ordered permutations of n elements. Quasi-free states allow to formulate the Hadamard property as a constraint on the singular structure of the associated ω_2:

Definition 2.6 A quasi-free state $\omega : \mathcal{F}(M) \to \mathbb{C}$ is called **Hadamard** if the associated two-point function $\omega_2 \in \mathcal{D}'(M \times M)$ is such that its wavefront set has the following form:

$$WF(\omega_2) = \left\{(x, y, k_x, -k_y) \in T^*M^2 \setminus \{\mathbf{0}\} \mid (x, k_x) \sim (y, k_y),\ k_x \rhd 0\right\}. \tag{6}$$

Here $(x, k_x) \sim (y, k_y)$ implies that there exists a null geodesic c connecting x to y such that k_x is coparallel and cotangent to c at x and k_y is the parallel transport of k_x from x to y along c. Finally, $k_x \rhd 0$ means that the covector k_x is future-directed.

Unfortunately Definition 2.6 is not constructive and, thus, one might wonder how to build concretely examples of Hadamard states. For many years only abstract

existence results via deformation techniques [20], or examples like the Poincaré vacuum and the Bunch-Davies state respectively on Minkowski and on the de Sitter spacetime were known. Yet, in the last decade, many novel construction schemes for Hadamard states, applicable in different frameworks, were devised. In the next section, we shall review one of them which is especially suited for those linear field theories built on globally hyperbolic spacetimes possessing a null (conformal) boundary.

2.1 Hadamard States from Null Infinity – I

In this section, we outline a procedure to construct explicitly Hadamard states, sometimes known as bulk-to-boundary correspondence. We will not work in full generality and we will be interested only in a massless, conformally coupled real scalar field, that is the dynamics is ruled by (1) with $m = 0$ and $\xi = \frac{1}{6}$. It is important to remark once more that the procedure, that we outline can be and has been applied to a wider range of free fields and of curved backgrounds, as we have already mentioned in the introduction. Since a full account of all these results would require much more space than that at our disposal, we start by reviewing the first application of this construction method, as it appeared in [11, 28, 29].

In particular, as starting point, we focus our attention on a particular class of globally hyperbolic spacetimes which are distinguished since they possess an asymptotic behavior along null directions which mimics that of Minkowski spacetime. Used extensively and successfully in the definition of black hole regions [34], the most general class of asymptotically flat spacetimes includes several important physical examples, such as for instance the Schwarzschild and the Kerr solutions to Einstein's equations. Here we employ the definition of asymptotic flatness, as introduced by Friedrich in [19]. To wit, we consider an **asymptotically flat spacetime with future timelike infinity** i^+, i.e., a globally hyperbolic spacetime (M, g), hereby called *physical spacetime*, such that there exists a second globally hyperbolic spacetime $(\widetilde{M}, \tilde{g})$, called *unphysical spacetime*, with a preferred point $i^+ \in \widetilde{M}$, a diffeomorphism $\Phi : M \to \Phi(M) \subset \widetilde{M}$ and a function $\Xi : \Phi(M) \to (0, \infty)$ so that $\Phi^*(\Xi^{-2}\tilde{g}) = g$. Furthermore, the following requirements ought to be satisfied:

(a) If we call $J^-_{\widetilde{M}}(i^+)$ the causal past of i^+, this is a closed set such that $\Phi(M) = J^-_{\widetilde{M}}(i^+) \setminus \partial J^-_{\widetilde{M}}(i^+)$ and we have $\partial M = \partial J^-_{\widetilde{M}}(i^+) = \mathscr{I}^+ \cup \{i^+\}$, where $\mathscr{I}^+$ is called *future null infinity*.

(b) Ξ can be extended to a smooth function on the whole $\widetilde{M}$ and it vanishes on $\mathscr{I}^+ \cup \{i^+\}$. Furthermore, $d\Xi \neq 0$ on $\mathscr{I}^+$ while $d\Xi = 0$ on i^+ and $\widetilde{\nabla}_\mu \widetilde{\nabla}_\nu \Xi = -2\,\tilde{g}_{\mu\nu}$ at i^+.

(c) Introducing $n^\mu \doteq \widetilde{\nabla}^\mu \Xi$, there exists a smooth and positive function ξ supported at least in a neighborhood of $\mathscr{I}^+$ such that $\widetilde{\nabla}_\mu(\xi^4 n^\mu) = 0$ on $\mathscr{I}^+$ and the integral curves of $\xi^{-1} n$ are complete on future null infinity.

Notice that we shall, henceforth, identify M with $\Phi(M)$. Here $\widetilde{\nabla}$ is the Levi-Civita connection built out of $\tilde{g}$. In the above definition, future timelike infinity plays a distinguished role, contrary to what happens in the more traditional definition of asymptotically flat spacetimes where i^+ is replaced by i_0, spatial infinity – see for example [34, Section 11]. The reason for our choice is motivated by physics: We are interested in working with the algebra $\mathcal{F}(M)$ of Definition 2.3 which is constructed out of E, the causal propagator associated to the operator P as in (1) with $m = 0$ and $\xi = \frac{1}{6}$. This entails in particular that, for any smooth and compactly supported function f, its image under the action of the causal propagator is supported in the causal future and past of $\mathrm{supp}(f)$. Therefore, it will be important in our investigation that future timelike infinity is actually part of the unphysical spacetime, so to be able to control the behavior of $E(f)$ thereon. Such requirement can be relaxed particularly if one is interested in studying field theories on manifolds like the Kruskal extension of Schwarzschild where i^+ cannot be made part of the unphysical spacetime. The price to pay in this case is the necessity to make sure that any solution of the classical dynamics falls off sufficiently fast as it approaches future timelike infinity. This line of reasoning has been pursued in [14], though we shall not follow it here since it relies heavily on the fact that a very specific manifold has been chosen. On the contrary, we work with a large class of backgrounds.

Before proceeding toward the construction of a Hadamard state for a massless, conformally coupled, real scalar field on a globally hyperbolic and asymptotically flat spacetime, we point out a few distinguished properties of future null infinity – see [28, 34] and references therein:

- $\mathscr{I}^+$ is a three dimensional, null submanifold of $\widetilde{M}$, diffeomorphic to $\mathbb{R} \times \mathbb{S}^2$. Furthermore, there exists an open neighborhood U of $\widetilde{M}$ containing $\mathscr{I}^+$ and a coordinate system $(u, \Xi, \theta, \varphi)$, called *Bondi chart*, such that (θ, φ) are the standard coordinates on the unit 2-sphere, u is an affine parameter along the null geodesic generating $\mathscr{I}^+$, while Ξ is the conformal factor, promoted to coordinate. In this system $\mathscr{I}^+$ is the locus $\Xi = 0$ and the line elements reads

$$ds^2\big|_{\mathscr{I}^+} = -2dud\Xi + d\theta^2 + \sin^2\theta d\varphi^2.$$

- There exists a distinguished subgroup of $Diff(\mathscr{I}^+)$, called the *Bondi-Metzner-Sachs (BMS) group*, which can be defined via its action on a Bondi frame: If $(z, \bar{z})$ are the complex coordinates built out of (θ, φ) via a stereographic projection,

$$\begin{cases} u \mapsto u' \doteq K_\Lambda(z, \bar{z})\,(u + \alpha(z, \bar{z})) \\ z \mapsto z' = \frac{az+b}{cz+d}, \quad ad - bc = 1, \quad \text{and c.c.}, \end{cases} \tag{7}$$

  where $a, b, c, d \in \mathbb{C}$, $\alpha \in C^\infty(\mathbb{S}^2)$,

$$\Lambda = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \quad \text{and} \quad K_\Lambda(z, \bar{z}) = \frac{1 + |z|^2}{|az + b|^2 + |cz + d|^2}. \tag{8}$$

By direct inspection, it turns out that (7) identifies the semidirect product $SL(2,\mathbb{C}) \ltimes C^\infty(\mathbb{S}^2)$. Notice that the BMS group coincides, moreover, with the group of asymptotic symmetries of the physical spacetime (M, g) [24].

We have all the ingredients to implement the bulk-to-boundary correspondence mentioned at the beginning of the section. The procedure is based on two key structures. First of all, one defines on top of $\mathscr{I}^+$ a symplectic space of functions and an associated $*$-algebra of fields. Secondly, one looks for an injective $*$-homomorphism from $\mathcal{F}(M)$, the algebra of fields defined in the physical spacetime (M, g), and the one on $\mathscr{I}^+$. As a byproduct of such homomorphism, every algebraic state on the boundary induces via pull-back a bulk counterpart. The net advantage is the fact that, at a geometric level, future null infinity comes endowed with the BMS group, which is an infinite dimensional symmetry group, which, exactly as the Poincaré group in Minkowski spacetime, allows to identify a distinguished ground state.

In order to implement this program, let us define:

$$\mathcal{S}(\mathscr{I}^+) \doteq \left\{\psi \in C^\infty(\mathscr{I}^+) \mid \psi \text{ and } \partial_u\psi \in L^2(\mathscr{I}^+, d\mu_{\mathscr{I}})\right\}, \tag{9}$$

where $d\mu_{\mathscr{I}} = \sin\theta du d\theta d\varphi$. This is a symplectic space if endowed with

$$\sigma_{\mathscr{I}} : \mathcal{S}(\mathscr{I}^+) \times \mathcal{S}(\mathscr{I}^+) \to \mathbb{R},\ (\psi, \psi') \mapsto \sigma_{\mathscr{I}}(\psi, \psi') = \int_{\mathscr{I}} d\mu_{\mathscr{I}} \left(\psi \partial_u \psi' - \psi' \partial_u \psi\right).$$

Following the same procedure used starting from $\mathcal{E}^{obs}(M)$ in (5),

Definition 2.7 We call $*$-*algebra of fields on* $\mathscr{I}^+$, $\mathcal{F}(\mathscr{I}^+) = \frac{\mathcal{T}(\mathscr{I}^+)}{\mathcal{I}(\mathscr{I}^+)}$, where

$$\mathcal{T}(\mathscr{I}^+) \doteq \bigoplus_{n=0}^{\infty} \mathcal{S}(\mathscr{I}^+; \mathbb{C})^{\otimes n}.$$

Here $\mathcal{S}(\mathscr{I}^+; \mathbb{C}) = \mathcal{S}(\mathscr{I}^+) \otimes \mathbb{C}$ whereas $\mathcal{S}(\mathscr{I}^+; \mathbb{C})^{\otimes 0} \doteq \mathbb{C}$. $\mathcal{I}(\mathscr{I}^+)$ is the $*$-ideal generated by the relation $\psi \otimes \psi' - \psi' \otimes \psi - i\sigma_{\mathscr{I}}(\psi, \psi')\mathbb{I}$, where $\mathbb{I}$ is the identity in $\mathcal{T}(\mathscr{I}^+)$. The $*$-operation is complex conjugation.

At this stage it becomes clear why we chose to work only with a massless, conformally coupled real scalar field. Since we want to construct a $*$-homomorphism between $\mathcal{F}(M)$ and $\mathcal{F}(\mathscr{I}^+)$, compatibility between the canonical commutation relations in $\mathcal{I}(M)$ and those in $\mathcal{I}(\mathscr{I}^+)$ suggest that we should start from an injective symplectomorphism between $(\mathcal{E}^{obs}(M), \sigma)$ and $(\mathcal{S}(\mathscr{I}^+), \sigma_{\mathscr{I}})$. In order to relate an equivalence class of compactly supported functions in M and a smooth function on $\mathscr{I}^+$, the procedure calls for propagating the former to null infinity via the causal propagator E associated to the underlying dynamics. Yet, one needs to remember that $\mathscr{I}^+$ is a submanifold of the unphysical spacetime which is related to the

physical one by a conformal transformation. In this respect it is a well-known fact that (1) is not well-behaved under such map, leading to pathological behaviors at $\mathscr{I}^+$ if a mass term or a coupling different from $\xi = \frac{1}{6}$ is present. On the contrary, as the name conformal coupling suggests, a solution to the massless and conformally coupled Klein-Gordon on (M, g) has the property of staying a solution of the same equation on $(\widetilde{M}, \tilde{g})$ up to a conformal rescaling. More precisely, the following holds true – see for example [11, 34]:

Proposition 2.8 *Let (M, g) be a globally hyperbolic and asymptotically flat spacetime, whose associated unphysical spacetime $(\widetilde{M}, \tilde{g})$, $\tilde{g}|_M = \Xi^2 g$, is also globally hyperbolic. Let R and $\widetilde{R}$ be the Ricci scalars built out of g and $\tilde{g}$ respectively. If ϕ is a smooth and spacelike compact solution of $P\phi = (\Box_g - \frac{R}{6})\phi$ on (M, g), $\widetilde{\phi} = \Xi^{-1}\phi$ is a solution of $\widehat{P}\widetilde{\phi} = \big(\Box_{\tilde{g}} - \frac{\widetilde{R}}{6}\big)\widetilde{\phi} = 0$ on $(M, \tilde{g})$. Furthermore, if $f \in C_0^\infty(M)$ is such that $\phi = E(f)$, E being the causal propagator of P, then $\widetilde{\phi} = \widetilde{E}_{\widehat{P}}(\Xi^{-3} f)\big|_M$, $\widetilde{E}_{\widehat{P}}$ being the causal propagator of $\widehat{P}$.*

As a byproduct of this last proposition, we have associated to every observable in the physical spacetime a spacelike compact smooth solution of the massless, conformally coupled Klein-Gordon equation on $(\widetilde{M}, \tilde{g})$. Due to the support properties of the causal propagator, every such solution can be restricted to $\mathscr{I}^+$, which is a smooth submanifold of $\widetilde{M}$. The relevant map is

$$\Upsilon : \mathcal{E}^{obs}(M) \to C^\infty(\mathscr{I}^+) \quad [f] \mapsto E_{\widehat{P}}(\Xi^{-3} f)\big|_{\mathscr{I}^+} . \tag{10}$$

As proven in [28, 29] the following key property holds true:

Proposition 2.9 *The application Υ, constructed in (10), is an injective linear map from $\mathcal{E}^{obs}(M)$ to $\mathcal{S}(\mathscr{I}^+)$ which is, moreover, a symplectomorphism. In other words, for every $[f], [f'] \in \mathcal{E}^{obs}(M)$*

$$\sigma\left([f], [f']\right) = \sigma_{\mathscr{I}}\left(\Upsilon([f]), \Upsilon([f'])\right),$$

where σ and $\sigma_{\mathscr{I}}$ are respectively the bulk and the boundary symplectic forms.

Notice that this proposition allows us to extend the action of the projection map Υ at a level of algebra of fields. On the one hand, we have automatically built a map from $\mathcal{T}(M)$ to $\mathcal{T}(\mathscr{I}^+)$, since Υ projects classical linear observables to elements in $\mathcal{S}(\mathscr{I}^+)$ which are respectively the generating space for the bulk and for the boundary universal tensor algebra. On the other hand, since Υ preserves at the same time the symplectic form, such map is compatible with the ideal generated by the canonical commutation relations on M and by $\sigma_{\mathscr{I}}$ on $\mathscr{I}^+$. Since the $*$-operation is complex conjugation both in the bulk and in the boundary and since Υ leaves it untouched, we have the following lemma:

Lemma 2.10 *There exists an injective $*$-homomorphism $\iota : \mathcal{F}(M) \to \mathcal{F}(\mathscr{I}^+)$ which is defined by its action on the generators, namely $\iota([f]) \doteq \Upsilon([f])$, $[f] \in \mathcal{E}^{obs}(M) \subset \mathcal{F}(M)$, where Υ is the map (10).*

The most important consequence of this lemma is the following: Let $\omega_{\mathscr{I}} : \mathcal{F}(\Im^+) \to \mathbb{C}$ be a normalized, positive linear functional, then

$$\omega \doteq \iota^* \omega_{\mathscr{I}} : \mathcal{F}(M) \to \mathbb{C}, \quad a \mapsto \omega(a) \doteq (\iota^* \omega_{\mathscr{I}})(a) = \omega_{\mathscr{I}}(\iota(a)), \ \forall\, a \in \mathcal{F}(M),$$

is a state for the algebra of fields on (M, g).

As a consequence, we can focus our attention on constructing algebraic states directly on null infinity, studying only subsequently the properties of the bulk counterpart, obtained via pull-back. As mentioned before, the advantage is the presence of the infinite dimensional BMS group on $\mathscr{I}^+$. Hence, the best course of action is to build a quasi-free/Gaussian state for $\mathcal{F}(\mathscr{I}^+)$ by looking for a BMS invariant two-point function on future null infinity. This problem has been discussed thoroughly in different publications [14, 28, 29] and we report here the main results:

Theorem 2.11 *Let* $\omega_{2,\mathscr{I}} : \mathcal{S}(\mathscr{I}^+) \otimes \mathcal{S}(\mathscr{I}^+) \to \mathbb{C}$ *be*

$$\omega_{2,\mathscr{I}}(\psi \otimes \psi') = -\frac{1}{\pi} \lim_{\epsilon \to 0} \int_{\mathbb{R}^2 \times \mathbb{S}^2} du du' d\mathbb{S}^2(\theta, \varphi) \frac{\psi(u, \theta, \varphi)\psi'(u', \theta, \varphi)}{(u - u' - i\epsilon)^2},$$

where $d\mathbb{S}^2(\theta, \varphi)$ *is the standard measure on the unit* 2*-sphere. Then the following holds true:*

1. $\omega_{2,\mathscr{I}}$ *defines a quasi-free state* $\omega_{\mathscr{I}}$ *for* $\mathcal{F}(\Im^+)$*. In its folium this is the unique BMS invariant state.*
2. *The state* $\omega \doteq \iota^* \omega_{\mathscr{I}} : \mathcal{F}(M) \to \mathbb{C}$ *is a quasi-free state for the algebra of fields in the bulk which is*
   - *of Hadamard form,*
   - *invariant under the action of all isometries of* (M, g).

Notice that invariance under all bulk isometries implies that our construction, applied to Minkowski spacetime, yields the Poincaré vacuum.

3 Linearized Gravity

The bulk-to-boundary correspondence, described in the previous section for a massless, conformally coupled real scalar field, can be applied to other free fields and to other globally hyperbolic spacetimes possessing a null boundary. Barring minor technical details, the procedure is always the same except when one deals with non-interacting gauge theories, since one needs to control additionally the gauge fixing. There are two cases which are certainly of relevance at a physical level: free electromagnetism and linearized gravity. The first was discussed a couple of years ago in [10], while the second was only analyzed last year and, therefore, we review it here, pointing out in particular the additional difficulties compared to

the scalar case. We will summarize mainly the results of [6] and of [17]. As in the previous sections, for the lack of space, we prefer to avoid giving the proofs of our statements, each time referring a reader to the relevant literature.

We consider still an arbitrary, globally hyperbolic and asymptotically flat spacetime (M, g) with the additional constraint that the Ricci tensor vanishes, $Ric(g) = 0$. In other words (M, g) is a solution of the Einstein vacuum equations. On top of (M, g) we consider a smooth symmetric 2-tensor $h \in \Gamma(S^2T^*M)$, where $S^2T^*M \doteq T^*M \otimes_s T^*M$, the subscript s standing for symmetrization. Dynamics is ruled by the linearized Einstein equations:

$$(Kh)_{ab} \doteq -\frac{g_{ab}}{2}\left(\nabla^c\nabla^d h_{cd} - \Box \mathrm{Tr}(h)\right) - \Box\frac{h_{ab}}{2} - \frac{1}{2}\nabla_a\nabla_b \mathrm{Tr}(h) + \nabla^c\nabla_{(a}h_{b)c} = 0, \tag{11}$$

where the indices are raised and lowered with the background metric. The symbol $\mathrm{Tr}(h)$ stands for $g^{ab}h_{ab}$, while the round brackets indicate a symmetrization with respect to the relevant indices, including the prefactor $\frac{1}{2}$.

Notice that, in this section, we will alternate between a notation where indices are explicit and one where they are implicit. This choice is related to our desire to avoid whenever possible a heavy notation where multiple subscripts appear.

As much as Einstein's theory comes together with invariance under the action of the diffeomorphism group, so (11) comes endowed with the linear counterpart. In other words two solutions h, h' of (11) are said to be gauge equivalent if there exists $\chi \in \Gamma(T^*M)$ such that

$$h' = h + \nabla_S \chi,$$

where $(\nabla_S \chi)_{ab} \doteq \nabla_{(a}\chi_{b)}$. Per direct inspection, one can realize that the operator K in (11) is not normally hyperbolic and, thus, one cannot construct smooth solutions using Green operators. Yet, one must keep in mind that, in gauge theories, we are not interested in single smooth solutions but actually in gauge equivalence classes of solutions. Hence, one can start from (11) and look for a gauge transformation which reduces the dynamics to that ruled by a normally hyperbolic operator or by one which at least admits Green operators. The following proposition shows that it is indeed possible – see for example [17]:

Proposition 3.1 *Let*

$$\mathcal{S}_K(M) = \left\{h \in \Gamma(S^2T^*M) \mid Kh = 0\right\}$$

be the space of smooth solutions to (11) *and let*

$$\mathcal{G}(M) = \left\{h \in \Gamma(S^2T^*M) \mid \exists \chi \in \Gamma(T^*M) \text{ for which } h = \nabla_S\chi\right\}.$$

Then, for every $[h] \in \frac{\mathcal{S}_K(M)}{\mathcal{G}}$*, there exists a representative* $\tilde{h}$ *such that*

$$\begin{cases} \widetilde{P}\tilde{h} = (\Box - 2Riem)\,(I\tilde{h}) = 0 \\ div(I\tilde{h}) = 0 \end{cases}, \tag{12}$$

where Riem is the Riemann tensor built out of g, I is the trace reversal operator such that $(I\tilde{h})_{ab} = \tilde{h}_{ab} - \frac{g_{ab}}{2} Tr(\tilde{h})$ *while div is the divergence operator such that* $(div(\tilde{h}))_b = \nabla^a \tilde{h}_{ab}$.

In this last proposition, we have introduced the standard de Donder gauge and it is noteworthy since $\widetilde{P}$ is manifestly the composition of a normally hyperbolic operator with a trace reversal. Hence, adapting Definitions 2.1 and 2.2 to the case at hand, we associate to $\widetilde{P}$ the advanced $(-)$ and the retarded $(+)$ fundamental solutions $G^{\pm}_{\widetilde{P}} \doteq G^{\pm}_{\Box - 2Riem} \circ I : \Gamma_{tc}(S^2T^*M) \to \Gamma(S^2T^*M)$ which have the properties that, for every $\beta \in \Gamma_{tc}(S^2T^*M)$

$$(\widetilde{P} \circ G^{\pm}_{\widetilde{P}})(\beta) = \beta = (G^{\pm}_{\widetilde{P}} \circ \widetilde{P})(\beta),$$

$$\mathrm{supp}(G^{\pm}_{\widetilde{P}}(\beta)) \subseteq J^{\pm}(\mathrm{supp}(\beta)).$$

Notice that $G^{\pm}_{\Box - 2Riem}$ stands for the advanced/retarded fundamental solution of the normally hyperbolic operator $\Box - 2Riem$. Additionally, we call $G_{\widetilde{P}} = G^{-}_{\widetilde{P}} - G^{+}_{\widetilde{P}}$ the *causal propagator of* $\widetilde{P}$. Yet, contrary to the scalar case, we cannot use only $G_{\widetilde{P}}$ to characterize in a covariant way the space of solutions of linearized gravity since we need also to take into account two additional data. On the one hand, there is the gauge-fixing condition $\mathrm{div}(I\tilde{h}) = 0$. This can be implemented by suitably restricting the space of admissible initial data, or more appropriately the admissible smooth and timelike compact sections of S^2T^*M, exploiting that $\mathrm{div} \circ I \circ G^{\pm}_{\widetilde{P}} = G^{\pm}_{\Box} \circ \mathrm{div}$, where $G^{\pm}_{\Box}$ are the advanced $(-)$ and the retarded $(+)$ Green operators for the d'Alembert wave operator acting on $\Gamma(T^*M)$. On the other hand, (12) is not a complete gauge fixing. As a matter of fact, if $\tilde{h}$ is a solution of (12), so is every $\tilde{h}'$ such that $\tilde{h}' - \tilde{h} = \nabla_S \chi$, $\chi \in \Gamma(T^*M)$ and $\Box\chi = 0$. Using this additional data, one can prove the following [6, 17]:

Proposition 3.2 *There exists an isomorphism between* $\frac{\mathcal{S}_K(M)}{\mathcal{G}(M)}$ *and* $\frac{Ker_{tc}(div)}{Im_{tc}(K)}$ *where* $Ker_{tc}(div) = \{\beta \in \Gamma_{tc}(S^2T^*M) \mid div(\beta) = 0\}$ *and* $Im_{tc}(K) = \{\beta \in \Gamma_{tc}(S^2T^*M) \mid \beta = K(\beta'),\ \beta' \in \Gamma_{tc}(S^2T^*M)\}$. *The isomorphism is realized by the causal propagator via* $[\beta] \in \frac{Ker_{tc}(div)}{Im_{tc}(K)} \mapsto [G(\beta)] \in \frac{\mathcal{S}_K(M)}{\mathcal{G}(M)}$.

Having under control the space of dynamical configurations for linearized gravity we can proceed to introducing classical linear observables along the same lines as in Sect. 2. There are two important differences which we shall point out. First of all, we start from all *kinematical configurations* $\Gamma(S^2T^*M)$ and, for every $\epsilon \in \Gamma_0(S^2TM)$,

we define the linear functional

$$\mathcal{O}_\epsilon : \Gamma(S^2T^*M) \to \mathbb{R}, \quad h \mapsto \mathcal{O}_\epsilon(h) = (\epsilon, h) \doteq \int_M d\mu_g \epsilon^{ab} h_{ab}. \tag{13}$$

The map $\mathcal{O}_\epsilon$ plays the role of a classical observable for kinematical configurations. At this stage comes the first difference from the scalar case, namely we need to encode the information of gauge invariance. This can be done by restricting our attention to those functionals of the form (13) which vanish on all pure gauge configurations, that is those $h \in \Gamma(S^2T^*M)$ such that $h = \nabla_S \chi$, $\chi \in \Gamma(T^*M)$. Using (13) and integration by parts, this entails

$$\mathcal{O}_\epsilon(\nabla_S \chi) = (\epsilon, \nabla_S \chi) = (\mathrm{div}(\epsilon), \chi) = 0.$$

The arbitrariness of χ and the non-degenerateness of the pairing $(,)$ entails that $\mathrm{div}(\epsilon) = 0$. In other words, we can introduce the space of gauge invariant functionals

$$\mathcal{L}^{inv}(M) = \{\mathcal{O}_\epsilon : \Gamma(S^2T^*M) \to \mathbb{R}, \mid \mathrm{div}(\epsilon) = 0, \epsilon \in \Gamma_0(S^2TM)\}.$$

As last step, we need to account for dynamics which can be done by restricting the domain of definition of the observables from $\Gamma(S^2T^*M)$ to $\mathcal{S}_K(M)$. Identifying once more the space of linear observables with its labeling space, hence, $\mathcal{L}^{inv}(M)$ with $Ker_0(\mathrm{div}) = \{\epsilon \in \Gamma_0(S^2TM) \mid \mathrm{div}(\epsilon) = 0\}$, the above restriction entails that $Ker_0(\mathrm{div})$ includes redundant observables which we need to quotient. As shown in [6] this is tantamount to defining the following as the space of *classical observables for linearized gravity*:

$$\mathcal{L}^{obs}(M) \doteq \frac{\mathcal{L}^{inv}(M)}{Im_0(K)}, \tag{14}$$

where $Im_0(K) = \{\epsilon \in \Gamma_0(S^2TM) \mid \epsilon = K(\alpha), \ \alpha \in \Gamma_0(S^2TM)\}$. Notice the second big difference from the scalar case. While $\mathcal{E}^{obs}(M)$ could be endowed with a symplectic form, this is not necessarily the case for $\mathcal{L}^{obs}(M)$, to which we can associate the following pre-symplectic form:

$$\tau : \mathcal{L}^{obs}(M) \times \mathcal{L}^{obs}(M) \to \mathbb{R}, \quad ([\epsilon], [\epsilon']) \mapsto (\epsilon, G_{\widetilde{P}})(\epsilon'^\flat), \tag{15}$$

where $G_{\widetilde{P}}$ is the causal propagator of $\widetilde{P}$, while $^\flat$ is the canonical, metric-induced musical isomorphism. It is important to stress that it is known that τ is non-degenerate if the Cauchy surface of M is compact – see for example [17] – or on Minkowski spacetime – see [26]. To the best of our knowledge, in all other cases the problem is still open.

Having chosen a space of classical observables entails that we can define a $*$-algebra of observables associated to the quantum theory.

Definition 3.3 We call **algebra of fields** for linearized gravity, the quotient $\mathcal{F}_{grav}(M) = \frac{\mathcal{T}_{grav}(M)}{\mathcal{I}_{grav}(M)}$. Here

$$\mathcal{T}_{grav}(M) \doteq \bigoplus_{n=0}^{\infty} \mathcal{L}^{obs}(M;\mathbb{C})^{\otimes n},$$

is the universal tensor algebra endowed with complex conjugation as $*$-operation, where $\mathcal{L}^{obs}(M;\mathbb{C}) = \mathcal{L}^{obs}(M)\otimes\mathbb{C}$ while $\mathcal{L}^{obs}(M;\mathbb{C})^{\otimes 0} \doteq \mathbb{C}$. $\mathcal{I}_{grav}(M)$ is the $*$-ideal generated by the *canonical commutation relations* $[\epsilon]\otimes[\epsilon']-[\epsilon']\otimes[\epsilon]-i\tau\,([\epsilon],[\epsilon'])\,\mathbb{I}$, where $\mathbb{I}$ is the identity in $\mathcal{T}_{grav}(M)$ and τ is defined in (15).

Notice that, since τ is not known to be symplectic, we cannot conclude that $\mathcal{F}_{grav}(M)$ is semisimple. Hence, it might contain an Abelian ideal, namely there might exist observables behaving classically regardless of the state chosen for $\mathcal{F}_{grav}(M)$. Furthermore, one can also show that $\mathcal{F}_{grav}(M)$ satisfies the counterpart of Proposition 2.4 for $\mathcal{F}(M)$: causality and the time-slice axiom. We will not enter into the details to avoid useless repetitions. The next step in our construction will be the identification of algebraic states of physical interest for linearized gravity. While the definition of an algebraic state and the content of Theorem 2.5 are left unchanged, the Hadamard condition requires to be slightly adapted to account for gauge invariance. More precisely, since we will be mainly interested in Gaussian states for $\mathcal{F}_{grav}(M)$, we will be looking for two-point functions $\omega_2 : \mathcal{L}^{obs}(M)\otimes\mathcal{L}^{obs}(M) \to \mathbb{R}$. In view of (14), this is tantamount to building $\Omega_2 : \mathcal{L}^{inv}(M)\otimes\mathcal{L}^{inv}(M) \to \mathbb{R}$, weak bi-solution of (11). Yet, since, on account of gauge invariance, $\mathcal{L}^{inv}(M)$ includes only those $\epsilon \in \Gamma_0(S^2TM)$ which are divergence free, we cannot ensure automatically that Ω_2 identifies a bi-distribution $\widetilde{\Omega}_2 : \Gamma_0(S^2TM)\times\Gamma_0(S^2TM) \to \mathbb{R}$. Additionally, we need to take into account that, besides $\widetilde{P}$, also the trace-reversal is present in (11). Following [17], we define a trace-reversal operation at the level of bi-distributions and, with a slight abuse of notation, we indicate it still with the letter I. Let thus $\widetilde{\Omega}_2$ be a bi-distribution on $\Gamma_0(S^2TM)$ we call *trace reversal* of $\widetilde{\Omega}_2$

$$I\widetilde{\Omega}_2 : \Gamma_0(S^2TM)\times\Gamma_0(S^2TM) \to \mathbb{R},$$

$$(\epsilon,\epsilon') \mapsto (I\widetilde{\Omega}_2)(\epsilon,\epsilon') = \widetilde{\Omega}_2(\epsilon,\epsilon') - \frac{1}{8}\mathrm{Tr}(\widetilde{\Omega}_2)(\mathrm{Tr}(\epsilon),\mathrm{Tr}(\epsilon')),$$

where $\mathrm{Tr}(\widetilde{\Omega}_2) \in \mathcal{D}'(M\times M)$ is defined as follows: for all $f, f' \in C_0^\infty(M)$,

$$\mathrm{Tr}(\widetilde{\Omega}_2)(f,f') \doteq \widetilde{\Omega}_2(g^{-1}f, g^{-1}f'),$$

g^{-1} being the inverse metric. To summarize [17]:

Definition 3.4 Let $\omega : \mathcal{F}_{grav}(M) \to \mathbb{C}$ be a quasi-free state. It is said to be **Hadamard** if there exists a bi-distribution $\widetilde{\Omega}_2 : \Gamma_0(S^2TM) \times \Gamma_0(S^2TM) \to \mathbb{R}$ which is a weak bi-solution of $\widetilde{P}$, its wavefront set has the same form of (6) and, for every $\epsilon, \epsilon' \in \mathcal{L}^{inv}(M)$,

$$\omega([\epsilon] \otimes [\epsilon']) = (I\widetilde{\Omega}_2)(\epsilon, \epsilon').$$

3.1 Hadamard States from Null Infinity – II

In this section, we will show how the bulk-to-boundary correspondence can be applied to linearized gravity. Hence, from now on (M, g) will indicate a globally hyperbolic, asymptotically flat spacetime with vanishing Ricci tensor and $(\widetilde{M}, \tilde{g})$ the associated unphysical spacetime. The most notable difference between a massless, conformally coupled real scalar field and linearized gravity consists of the behavior under a conformal transformation of the equations ruling the dynamics. As a matter of fact, by mapping g to $\Xi^2 g$, (11) transforms in such a way that several terms proportional to inverse powers of Ξ appear. Taking into account that the null boundary of an asymptotically flat spacetime is the locus $\Xi = 0$, such behavior is problematic. This feature is not present only for linearized gravity, but also for free electromagnetism, written in terms of the vector potential. The solution in all these cases is to exploit gauge invariance, namely to look for a suitable gauge fixing which makes the dynamics hyperbolic and, upon a conformal transformation, controls all possible divergences due to the terms proportional to inverse powers of Ξ. While, in free electromagnetism, the standard Lorenz gauge is the right choice, for linearized gravity, the de Donder gauge is not suitable for this task. The problem was tackled in the literature, especially in connection to the stability of asymptotically simple spacetimes and an answer was found going under the name of *Geroch-Xanthopoulos* gauge [25].

Let us now go into the details of the construction. As in the scalar case, the starting point is the identification of a suitable space of tensors living on future null infinity. Following [1], we define

$$\widetilde{\mathcal{S}}(\mathscr{I}^+) = \{\lambda \in \Gamma(S^2T^*\mathscr{I}^+) \mid \lambda_{ab}n^a = 0 \text{ and } \lambda_{ab}q^{ab} = 0\},$$

where $n_a = \widetilde{\nabla}_a \Xi$ and $\widetilde{\nabla}$ is the covariant derivative built out of $\tilde{g}$. The tensor $q = \iota^* g$ where $\iota : \mathscr{I}^+ \to \widetilde{M}$ and q^{ab} is any inverse such that $q^{ab}q_{ac}q_{bd} = q_{cd}$. Subsequently, we consider a vector subspace

$$\mathcal{S}_{grav}(\mathscr{I}^+) \doteq \{\lambda \in \widetilde{\mathcal{S}}(\mathscr{I}^+) \mid (\lambda, \lambda)_{\mathscr{I}} < \infty, \quad \text{and} \quad (\partial_u\lambda, \partial_u\lambda)_{\mathscr{I}} < \infty\},$$

where, for any $\lambda, \lambda' \in \widetilde{\mathcal{S}}(\mathscr{I}^+)$,

$$(\lambda, \lambda')_{\mathscr{I}} \doteq \int_{\mathscr{I}} d\mu_{\mathscr{I}} \lambda_{ab} \lambda'_{cd} q^{ac} q^{bd}.$$

As for the real scalar case, the space of functions on future null infinity has been chosen since it has two important properties:

1. It is a symplectic space if endowed with the following antisymmetric bilinear form:

$$\tau_{\mathscr{I}} : \mathcal{S}_{grav}(\mathscr{I}^+) \times \mathcal{S}_{grav}(\mathscr{I}^+) \to \mathbb{R},$$
$$(\lambda, \lambda') \mapsto \tau_{\mathscr{I}}(\lambda, \lambda') = \int_{\mathscr{I}} d\mu_{\mathscr{I}} (\lambda_{ab} \mathcal{L}_n \lambda'_{cd} - \lambda'_{ab} \mathcal{L}_n \lambda_{cd}) q^{ac} q^{bd}, \tag{16}$$

   where $\mathcal{L}_n$ is the Lie derivative along the vector field n on $\mathscr{I}^+$.
2. The pair $(\mathcal{S}_{grav}(\mathscr{I}^+), \tau_{\mathscr{I}})$ is invariant under the following representation Π of the BMS group (7): Let us fix a Bondi frame on $\mathscr{I}^+$, let $(\Lambda, \alpha(z, \bar{z})) \in$ BMS and let $\lambda \in \mathcal{S}_{grav}(\mathscr{I}^+)$; then, recalling (8),

$$\left[\Pi_{(\Lambda,\alpha)} \lambda\right](u, z, \bar{z}) = K_\Lambda(z, \bar{z}) \lambda(u + \alpha(z, \bar{z}), z, \bar{z}). \tag{17}$$

In view of these properties of the space of functions, which we use on future null infinity, we can define an auxiliary $*$-algebra on $\mathscr{I}^+$:

Definition 3.5 The *$*$-algebra of fields for linearized gravity on future null infinity is denoted by* $\mathcal{F}_{grav}(\mathscr{I}^+) = \frac{\mathcal{T}_{grav}(\mathscr{I}^+)}{\mathcal{I}_{grav}(\mathscr{I}^+)}$, where

$$\mathcal{T}_{grav}(\mathscr{I}^+) \doteq \bigoplus_{n=0}^{\infty} \mathcal{S}_{grav}(\mathscr{I}^+; \mathbb{C})^{\otimes n}.$$

Here $\mathcal{S}_{grav}(\mathscr{I}^+; \mathbb{C}) = \mathcal{S}_{grav}(\mathscr{I}^+) \otimes \mathbb{C}$ whereas $\mathcal{S}_{grav}(\mathscr{I}^+; \mathbb{C})^{\otimes 0} \doteq \mathbb{C}$. At the same time $\mathcal{I}_{grav}(\mathscr{I}^+)$ is the $*$-ideal generated by the relation $\lambda \otimes \lambda' - \lambda' \otimes \lambda - i\tau_{\mathscr{I}}(\lambda, \lambda')\mathbb{I}$, where $\mathbb{I}$ is the identity in $\mathcal{T}_{grav}(\mathscr{I}^+)$. The $*$-operation is complex conjugation.

The next step consists of associating to each classical linear observable in (M, g) an element of $\mathcal{S}_{grav}(\mathscr{I}^+)$. We follow again the procedure devised in [1]. First of all, we remark that, to every $[\epsilon] \in \mathcal{L}^{obs}(M)$, we can associate $E\widetilde{_P}(\epsilon^\flat)$, which is a smooth and spacelike compact solution of (12) and, thus, also of (11).

Definition 3.6 We call *classical radiative observables*, $\mathcal{L}^{rad}(M)$, the collection of all $[\epsilon] \in \mathcal{L}^{obs}(M)$, for which $E\widetilde{_P}(\epsilon^\flat)$ is gauge equivalent to a smooth and spacelike compact solution h of (11) in the **Geroch-Xanthopoulos gauge**, that is setting $\gamma_{ab} = \Xi \gamma'_{ab}$, $\gamma_a = \Xi^{-1} n^b \gamma'_{ab}$, $\gamma = \tilde{g}^{ab} \gamma_{ab}$ and $f = \Xi^{-1} n^a n_a$ and $n_a = \nabla_a \Xi = \widetilde{\nabla}_a \Xi$, it

holds that

$$y_a = \widetilde{\nabla}^b \gamma_{ab} - \widetilde{\nabla}_a \gamma - 3\gamma_a = 0, \tag{18a}$$

$$\left(n^a \widetilde{\nabla}_a + \frac{1}{6}\Xi \widetilde{R} + \frac{3}{2} f\right) \widetilde{\Box}\gamma = \frac{1}{12}\widetilde{R} f \gamma - \frac{1}{2}\gamma \widetilde{\Box} f - \frac{1}{3}\widetilde{R} n^a \gamma_a + \frac{4}{\Xi}\widetilde{C}_{abcd}\gamma^{bd} n^a n^c, \tag{18b}$$

where $\widetilde{\cdot}$ refers to quantities computed with respect to $\tilde{g}$, e.g., $\widetilde{C}_{abcd}$ is the Weyl tensor for $\tilde{g}$. At the same time, we call *algebra of radiative observables* $\mathcal{F}^{rad}(M)$ the $*$-subalgebra of $\mathcal{F}_{grav}(M)$ built out of $\mathcal{L}^{rad}(M)$.

Radiative observables play a distinguished role since, as shown in [1, 25], (11) in combination with the Geroch-Xanthopoulos gauge yields an hyperbolic system of partial differential equations on $(\widetilde{M}, \tilde{g})$. Thus, every $\gamma = \Xi h$, $h = E_{\widetilde{P}}(\epsilon^\flat)$ and $[\epsilon] \in \mathcal{L}^{rad}(M)$, can be uniquely extended to a smooth solution of the conformally transformed equations of motion for linearized gravity in the unphysical spacetime. More importantly such extension can be restricted to future null infinity and, as proven in [1, 6],

Proposition 3.7 *Let us endow $\mathcal{L}^{rad}(M)$ with the restriction of (15) thereon. Then, there exists a map $\Upsilon_{grav} : \mathcal{E}^{rad}(M) \to \mathcal{S}_{grav}(\mathscr{I}^+)$ such that, for all $[\epsilon], [\epsilon'] \in \mathcal{E}^{rad}(M)$,*

$$\tau_{\mathscr{I}}([\epsilon], [\epsilon']) = \tau(\Upsilon_{grav}([\epsilon]), \Upsilon_{grav}([\epsilon'])),$$

where $\tau_{\mathscr{I}}$ is defined in (16). Υ_{grav} can be extended to a $*$-homomorphism $\iota_{grav} : \mathcal{F}^{rad}(M) \to \mathcal{F}_{grav}(\mathscr{I}^+)$ which is completely defined by its action on the generators, namely, for every $[\epsilon] \in \mathcal{L}^{rad}(M)$, $\iota_{grav}([\epsilon]) \doteq \Upsilon_{grav}([\epsilon])$.

Notice that, contrary to the scalar case and due to our lack of control on the non-degenerateness of (15), we cannot conclude that ι_{grav} is injective. Yet, this is no obstacle for constructing states on $\mathcal{F}^{rad}(M)$ via a pull-back of those for $\mathcal{F}_{grav}(\mathscr{I}^+)$. Before investigating this problem, we need to answer an important question, namely if $\mathcal{L}^{rad}(M)$ coincides with $\mathcal{L}^{obs}(M)$. In the original paper [25], it appeared as if every smooth and spacelike compact solution of (11) could be transformed into one in the Geroch-Xanthopoulos gauge. Yet, a closer investigation of the procedure unveils the presence of obstructions. Most surprisingly it turns out that problems arise in implementing (18a) rather than (18b). More precisely, let $h \in \Gamma(S^2T^*M)$ be a solution of (11) and let $h' = h + \nabla_S \chi$, $\chi \in \Gamma(T^*M)$. Then, a direct computation shows that h' satisfies (18a) if and only if

$$\nabla^b \nabla_{[b}\chi_{a]} = -v_a(h), \quad v_a(h) \doteq \nabla^b h_{ab} - \nabla_a h,$$

where the square brackets between the subscripts stand for total antisymmetrization, including the prefactor $\frac{1}{2}$. This identity entails that $v \in \Gamma(T^*M)$ must be a co-exact

1-form, a property which is not obviously satisfied. In [6], the following has been proven:

Proposition 3.8 *Let $h = E_{\widetilde{P}}(\epsilon^\flat)$ with $[\epsilon] \in \mathcal{L}^{obs}(M)$. Then h is gauge equivalent to a solution of (11) if and only if $Tr(\epsilon) = g_{ab}\epsilon^{ab}$ is the codifferential of a compactly supported 1-form.*

Proposition 3.8 offers a more practical condition to verify the implementability of the Geroch-Xanthopoulos gauge, although the question is still non-trivial since one has to account for two mixing conditions, ϵ being divergence free and its trace being co-exact. Yet, in [6] it has been proven that, while on Minkowski spacetime the hypotheses of Proposition 3.8 are met, there exist asymptotically flat, globally hyperbolic and Ricci flat spacetimes for which they are not. Most notably it suffices that the Cauchy surface Σ of (M, g) is diffeomorphic to $X \times \mathbb{S}^1$, X being a codimension 1 submanifold of Σ and that g admits a Killing field along $\mathbb{S}^1$.

Having understood under which conditions radiative observables coincide with all classical linear ones, we can revert to our main investigation, namely the construction of Hadamard states. At this stage the procedure will be identical to the one described in Sect. 2.1 and we shall only sketch the key points. The starting one is Proposition 3.7 and in particular the $*$-homomorphism ι_{grav}. First of all, we identify a distinguished quasi-free state for $\mathcal{F}_{grav}(\mathscr{I}^+)$:

Proposition 3.9 *The map $\omega_2^\Im : \mathcal{S}_{grav}(\mathscr{I}^+;\mathbb{C}) \otimes \mathcal{S}_{grav}(\mathscr{I}^+;\mathbb{C}) \to \mathbb{R}$ is such that*

$$\omega_2^\Im(\lambda \otimes \lambda') = -\frac{1}{\pi} \lim_{\epsilon \to 0} \int_{\mathbb{R}^2 \times \mathbb{S}^2} \frac{\lambda_{ab}(u,\theta,\varphi)\lambda'_{cd}(u',\theta,\varphi)q^{ac}q^{bd}}{(u-u'-i\epsilon)^2}\, du\, du'\, d\mathbb{S}^2(\theta,\varphi), \tag{19}$$

where $d\mathbb{S}^2(\theta,\varphi)$ is the standard line element on the unit 2-sphere, unambiguously defines a quasi-free state $\omega^\Im : \mathcal{F}_{grav}(\mathscr{I}^+) \to \mathbb{C}$. Furthermore:

1. *$\omega^\Im$ induces via pull-back a quasi-free bulk state $\omega^M : \mathcal{F}^{rad}(M) \to \mathbb{C}$ such that $\omega^M \doteq \omega^\Im \circ \Upsilon$,*
2. *$\omega^\Im$ is invariant under the action Π of the BMS group induced by (17) on $\mathcal{F}_{grav}(\mathscr{I}^+)$.*

Notice that we use the symbol Π with a slight abuse of notation since we have already introduced it to indicate in (17) the representation of the BMS group on $\mathcal{S}(\mathscr{I}^+)$. Since $\mathcal{F}_{grav}(\mathscr{I}^+)$ is built out of $\mathcal{S}(\mathscr{I}^+)$, we feel that no confusion can arise. As a last step, we need to combine (19) with Definition 3.4 to conclude that, for all those asymptotically flat and globally hyperbolic spacetimes for which $\mathcal{E}^{obs}(M) = \mathcal{E}^{rad}(M)$, it holds – see [6] for the proof:

Theorem 3.10 *Let $\iota : \mathcal{F}^{rad}(M) \to \mathcal{F}_{grav}(\mathscr{I}^+)$ be as in Proposition 3.7. The state $\omega^M = \omega^\Im \circ \iota : \mathcal{F}^{rad}(M) \to \mathbb{C}$, where $\omega^\Im$ is the state introduced in Proposition 3.9, has the following properties:*

1. *Its two-point function is the restriction to* $\mathcal{E}^{rad}(M) \times \mathcal{E}^{rad}(M)$ *of a bi-distribution on* $\widetilde{M}$ *whose wavefront set on M, seen as an open submanifold of* $\widetilde{M}$*, is of Hadamard from.*
2. *It is invariant under the action of all isometries of the bulk metric g, that is* $\omega^M \circ \alpha_\phi = \omega^M$*. Here* $\phi : M \to M$ *is any isometry and* α_ϕ *represents the action of* ϕ *induced on* $\mathcal{F}^{rad}(M)$ *by setting* $\alpha_\phi([\epsilon]) = [\phi_* \epsilon]$ *on the algebra generators* $[\epsilon] \in \mathcal{E}^{rad}(M)$*.*
3. *It coincides with the Poincaré vacuum on Minkowski spacetime.*

Acknowledgements The author is grateful to the University of Regensburg and to the organizing committee for the kind hospitality during the workshop *Quantum Mathematical Physics* held from the 29th of September to 2nd of October 2014. C. D. is grateful to Simone Murro for the useful discussions.

References

1. A. Ashtekar, A. Magnon-Ashtekar, On the symplectic structure of general relativity. Commun. Math. Phys. **86**, 55–68 (1982)
2. C. Bär, Green-hyperbolic operators on globally hyperbolic spacetimes. Commun. Math. Phys. **333**, 1585–1615 (2015)
3. C. Bär, K. Fredenhagen, *Quantum Field Theory on Curved Spacetimes*. Lecture Notes in Physics, vol. 786 (Springer, Dordrecht/New York, 2009)
4. C. Bär, N. Ginoux, F. Pfäffle, *Wave Equations on Lorenzian Manifolds and Quantization* (European Mathematical Society, 2007)
5. M. Benini, C. Dappiaggi, T.-P. Hack, Quantum field theory on curved backgrounds – a primer. Int. J. Mod. Phys. A **28**, 1330023 (2013)
6. M. Benini, C. Dappiaggi, S. Murro, Radiative observables for linearized gravity on asymptotically flat spacetimes and their boundary induced states. J. Math. Phys. **55**, 082301 (2014)
7. M. Benini, Optimal space of linear classical observables for Maxwell k-forms via spacelike and timelike compact de Rham cohomologies. [arXiv:1401.7563 [math-ph]]
8. A.N. Bernal, M. Sanchez, Smoothness of time functions and the metric splitting of globally hyperbolic space-times. Commun. Math. Phys. **257**, 43–50 (2005)
9. M. Brum, S.E. Jorás, Hadamard state in Schwarzschild-de Sitter spacetime. Class. Quantum Gravity **32**, 015013 (2015)
10. C. Dappiaggi, D. Siemssen, Hadamard States for the vector potential on asymptotically flat spacetimes. Rev. Math. Phys. **25**, 1350002 (2013)
11. C. Dappiaggi, V. Moretti, N. Pinamonti, Rigorous steps towards holography in asymptotically flat spacetimes. Rev. Math. Phys. **18**, 349–416 (2006)
12. C. Dappiaggi, V. Moretti, N. Pinamonti, Cosmological horizons and reconstruction of quantum field theories. Commun. Math. Phys. **285**, 1129–1163 (2009)
13. C. Dappiaggi, V. Moretti, N. Pinamonti, Distinguished quantum states in a class of cosmological spacetimes and their Hadamard property. J. Math. Phys. **50**, 062304 (2009)
14. C. Dappiaggi, V. Moretti, N. Pinamonti, Rigorous construction and Hadamard property of the Unruh state in Schwarzschild spacetime. Adv. Theor. Math. Phys. **15**, 355–448 (2011)
15. C. Dappiaggi, T.-P. Hack, N. Pinamonti, Approximate KMS states for scalar and spinor fields in Friedmann-Robertson-Walker spacetimes. Ann. Henri Poincare **12**, 1449–1489 (2011)
16. C. Dappiaggi, N. Pinamonti, M. Porrmann, Local causal structures, Hadamard states and the principle of local covariance in quantum field theory. Commun. Math. Phys. **304**, 459–498 (2011)

17. C.J. Fewster, D.S. Hunt, Quantization of linearized gravity in cosmological vacuum spacetimes. Rev. Math. Phys. **25**, 1330003 (2013)
18. K. Fredenhagen, K. Rejzner, QFT on curved spacetimes: axiomatic framework and examples. arXiv:1412.5125 [math-ph].
19. H. Friedrich, On purely radiative space-times. Commun. Math. Phys. **103**, 35–65 (1986)
20. S.A. Fulling, F.J. Narcowich, R.M. Wald, Singularity structure of the two point function in quantum field theory in curved space-time. II. Ann. Phys. **136**, 243–272 (1981)
21. C. Gérard, M. Wrochna, Construction of Hadamard states by characteristic Cauchy problem. arXiv:1409.6691 [math-ph].
22. C. Gérard, M. Wrochna, Construction of Hadamard states by pseudo-differential calculus. Commun. Math. Phys. **325**, 713–755 (2014)
23. C. Gérard, M. Wrochna, Hadamard states for the linearized Yang-Mills equation on curved spacetime. Commun. Math. Phys. **337**(1), 253–320 (2015)
24. R.P. Geroch, Asymptotic Structure of Space-Time, in *Proceedings of the Symposium on Asymptotic Structure of Space-Time*, ed. by W. Esposito (Plenum Press, New York, 1977)
25. R.P. Geroch, B.C. Xanthopoulos, Asymptotic simplicity is stable. J. Math. Phys. **19**, 714–719 (1978)
26. T.-P. Hack, Quantization of the linearised Einstein-Klein-Gordon system on arbitrary backgrounds and the special case of perturbations in inflation. Class. Quantum Gravity **31**(21), 215004 (2014)
27. S. Hollands, R.M. Wald, Local Wick polynomials and time ordered products of quantum fields in curved space-time. Commun. Math. Phys. **223**, 289–326 (2001)
28. V. Moretti, Uniqueness theorem for BMS-invariant states of scalar QFT on the null boundary of asymptotically flat spacetimes and bulk-boundary observable algebra correspondence. Commun. Math. Phys. **268**, 727–756 (2006)
29. V. Moretti, Quantum out-states holographically induced by asymptotic flatness: invariance under spacetime symmetries, energy positivity and Hadamard property. Commun. Math. Phys. **279**, 31–75 (2008)
30. V. Moretti, *Spectral Theory and Quantum Mechanics : With an Introduction to the Algebraic Formulation* (Springer, Milan, 2013)
31. M.J. Radzikowski, Micro-local approach to the Hadamard condition in quantum field theory on curved space-time. Commun. Math. Phys. **179**, 529–553 (1996)
32. M.J. Radzikowski, A Local to global singularity theorem for quantum field theory on curved space-time. Commun. Math. Phys. **180**, 1–22 (1996)
33. K. Sanders, A note on spacelike and timelike compactness. Class. Quantum Gravity **30**, 115014 (2013)
34. R.M. Wald, *General Relativity* (Chicago University Press, Chicago, 1984)

Local Thermal Equilibrium States in Relativistic Quantum Field Theory

Michael Gransee

Contents

Abstract It is well-known that thermal equilibrium states in quantum statistical mechanics and quantum field theory can be described in a mathematically rigorous manner by means of the so-called Kubo-Martin-Schwinger (KMS) condition, which is based on certain analyticity and periodicity properties of correlation functions. On the other hand, the characterization of non-equilibrium states which only locally have thermal properties still constitutes a challenge in quantum field theory. We discuss a recent proposal for characterization of such states by a generalized KMS condition. The connection of this proposal to a proposal by D. Buchholz, I. Ojima and H.-J. Roos for characterizing local thermal equilibrium states in quantum field theory is discussed.

Keywords Thermal quantum field theory • Local thermal equilibrium • Quantum statistical mechanics

Mathematics Subject Classification (2010). 81T05; 81T28; 82C10

M. Gransee (✉)
Max Planck Institut für Mathematik in den Naturwissenschaften, Inselstrasse 22, 04103 Leipzig, Germany
e-mail: gransee@mis.mpg.de

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_6

1 Introduction

Soon after the introduction of the algebraic approach to quantum field theory, developed by Araki, Haag and Kastler in the 1960s [1, 15], it became clear that this framework allows for an immediate adoption to non-relativistic quantum systems, for example spin lattice models. This led to the conclusion that equilibrium states in quantum statistical mechanics should be described in the operator-algebraic framework by the Kubo-Martin-Schwinger (KMS) condition, which was first envisaged by Haag, Hugenholtz and Winnink in [16]. The mathematically rigorous formulation of equilibrium quantum statistical mechanics based on the KMS condition has offered many insights into the structural properties of equilibrium states and at the same time has revealed previously unexpected connections to pure mathematics, in particular to Tomita-Takesaki modular theory, which had a huge influence on the understanding of quantum field theory, see e.g. the review article of Borchers [3]. For references and an extensive discussion of non-relativistic quantum statistical mechanics in the operator algebraic formulation, the reader is referred to the monograph by Bratteli and Robinson [4]. Interestingly, it took almost 20 years until the KMS condition was used in the rigorous investigation of thermal properties of relativistic quantum fields. This was initiated by Buchholz and Junglas [8, 9], leading to a fully relativistic version of the KMS condition [5] and an axiomatic approach to thermal field theory (à la Wightman [25]), in which the relativistic spectrum condition is replaced by the relativistic KMS condition [6].

Although the KMS condition turned out to be fruitful in this respect, it is clear from the outset that, in general, an arbitrary state of a quantum system will not be an equilibrium (KMS) state, since in nature there also arises a variety of non-equilibrium states ranging from mild perturbations of equilibrium states to steady states (e.g. a steady heat flow through a metal bar) and hydrodynamic flows (for example water in a pipe), up to states which do not admit any thermal interpretation at all. On the side of relativistic QFT, Buchholz, Ojima and Roos [10] developed a method for distinguishing between states which are out of equilibrium but locally still have a thermodynamical interpretation. Heuristically speaking, a *local thermal equilibrium (LTE) state* is defined as a state for which certain (point-like) observables, representing intensive thermal quantities like temperature, pressure and thermal stress-energy, take the same values as they take if the quantum field is in some thermal reference state (a KMS state or a mixture of such). Below we will discuss how this can be made precise and review several aspects of the LTE condition in quantum field theory.

The KMS condition is based on given analyticity and periodicity properties of correlation functions and yields an *intrinsic* characterization of equilibrium states. In contrast, the LTE condition of Buchholz, Ojima and Roos has to be regarded an *extrinsic* condition, since it is based on the comparison of a state with the members of an a priori fixed family of thermal reference states. It seems to be natural to ask if one could characterize such local equilibrium states in a manner similar to the KMS condition, i.e. by an *intrinsic* condition also based on analyticity and

periodicity properties of the correlation functions of LTE states. In fact, recent results of Gransee, Pinamonti and Verch show that this is possible. Motivated by the analysis of correlation functions of KMS states of the free quantized scalar field, in [14] a generalized version of the KMS condition, called *local KMS* (LKMS) condition, is introduced. Following this, it is shown that a certain class of LTE states in the sense of [10] can be equivalently described by this condition. We will discuss the LKMS condition and its relation to the LTE condition in Sect. 3 below.

1.1 Preliminaries

The QFT model For simplicity we consider an uncharged free scalar quantum field on Minkowski spacetime $\mathbb{M} = \mathbb{R}^4$, with the Minkowski pseudo-metric η of diagonal form $\eta = \mathrm{diag}(+1, -1, -1, -1)$. The field is regarded as an operator-valued distribution $f \mapsto \phi(f)$ on the space $\mathcal{S}(\mathbb{M})$ of Schwartz functions f, where the operators are all defined on a common dense and stable domain $\mathcal{D}$ of the underlying Hilbert space $\mathcal{H}$. The algebra of local observables is the *-algebra $\mathcal{A}(\mathbb{M})$, generated by multiples of $\mathbb{1}$ and finite sums as well as products of the field operators. This algebra is stable under the action of the proper, orthochronous Poincaré group $\mathcal{P}^{\uparrow}_{+}$, implemented on the field operators by

$$\tau_{(\Lambda,a)}(\phi(f)) = \phi(f_{(\Lambda,a)}), \tag{1}$$

where $f_{(\Lambda,a)}(x) = f(\Lambda^{-1}(x-a))$, and stable under the action of the gauge group $\mathbb{Z}_2$, acting as $\gamma(\phi(f)) = -\phi(f)$. Furthermore, we assume that

(i) $f \mapsto \phi(f)$ is linear.
(ii) $\phi(f)^* = \phi(\bar{f})$ for all $f \in \mathcal{S}(\mathbb{M})$.
(iii) Klein Gordon equation: $\phi((\Box + m^2)f) = 0$ for all $f \in \mathcal{S}(\mathbb{M})$, where $\Box$ denotes the d'Alembert operator and $m \geq 0$ is the mass parameter.
(iv) Canonical Commutation Relations (CCR): $[\phi(f), \phi(g)] = iE(f,g)\mathbb{1}$ for all $f, g \in \mathcal{S}(\mathbb{M})$, where E denotes the causal propagator, which is defined as the difference of the advanced minus the retarded fundamental solution of the Klein-Gordon equation. Einstein causality is expressed by $E(f,g) = 0$ if f and g have mutually spacelike separated supports.

A *state on* $\mathcal{A}(\mathbb{M})$ is a continuous normalized positive linear functional $\omega : \mathcal{A}(\mathbb{M}) \to \mathbb{C}$. The n-point "functions" of a state are distributions in $\mathcal{S}'(\mathbb{M}^n)$, formally given by

$$\omega_n(x_1, \ldots, x_n) := \omega(\phi(x_1) \cdots \phi(x_n)), \quad n \in \mathbb{N}. \tag{2}$$

Mostly, we will focus on quasifree states which are determined by their two-point functions ω_2 through

$$\omega\left(e^{it\phi(f)}\right) = e^{-\frac{1}{2}\omega_2(f,f)\cdot t^2}, \tag{3}$$

where the equation is to interpreted as equating terms of equal order in t. Furthermore, we assume that the states are gauge invariant, which means $\omega \circ \gamma = \omega$.

In the following we will only consider (quasifree) states fulfilling the *Hadamard condition*, characterized by the following restriction on $\mathrm{WF}(\omega_2)$, the wave front set of their two-point functions,

$$\mathrm{WF}(\omega_2) = \{(x, x', k, -k) \in T^*\mathbb{M}^2 : x \sim_k x', k_0 > 0\}, \tag{4}$$

or even analytic Hadamard states, characterized by a restriction on the analytic wave-front set of their two-point functions:

$$\mathrm{WF}_A(\omega_2) = \{(x, x', k, -k) \in T^*\mathbb{M}^2 : x \sim_k x', k_0 > 0\}. \tag{5}$$

For a discussion of the properties and a definition, the reader is referred to [19, 26] and references therein. For a motivation why one would prefer to consider Hadamard states, see e.g. [2].

Definition 1.1 Let $\mathcal{A}$ be a *-algebra, α_t a one-parameter group of automorphisms on $\mathcal{A}$, ω a state on $\mathcal{A}$ and $\beta > 0$. Define the open strip S_β by $S_\beta := \{z \in \mathbb{C} : 0 < \Im z < \beta\}$ and denote by $\bar{S}_\beta$ the closed strip. Then ω is called a *KMS state at value β with respect to α_t* (or (β, α_t)-KMS state, for short), iff for any $A, B \in \mathcal{A}$ there exists a function $F_{A,B}$, which is defined and holomorphic on S_β, and continuous on $\bar{S}_\beta$, with boundary values

$$F_{A,B}(t) = \omega\left(A\alpha_t(B)\right), \tag{6}$$

$$F_{A,B}(t + i\beta) = \omega\left(\alpha_t(B)A\right), \tag{7}$$

for all $t \in \mathbb{R}$.

A Lorentz frame is fixed by the choice of a future-directed timelike unit vector e; this means $e \in V_+$, where V_+ denotes the open forward lightcone, and $e^2 \equiv e^\mu e_\mu = 1$. The set of those vectors will be denoted by V_+^1 in the following. In the present model the one-parameter group of time evolution on $\mathcal{A}(\mathbb{M})$ with respect to the Lorentz frame fixed by some $e \in V_+^1$ is given by

$$\alpha_t^{(e)} = \tau_{(1,te)}, \quad t \in \mathbb{R}. \tag{8}$$

A KMS state ω_β with respect to $\alpha_t^{(e_\beta)}$ is regarded as a thermal equilibrium state at inverse temperature β with respect to the rest system (or Lorentz frame) specified

by some $e_\beta \in V_+^1$. Therefore thermal equilibrium states in relativistic QFT are indicated by both inverse temperature β and time direction e_β of the rest system. It is convenient to combine the two quantities into the inverse temperature four-vector $\boldsymbol{\beta} = \beta e_\beta \in V_+$ so that $\omega_{\boldsymbol{\beta}}$ denotes a $(\beta, \alpha_t^{(e_\beta)})$-KMS state on $\mathcal{A}(\mathbb{M})$. We therefore call $\omega_{\boldsymbol{\beta}}$ simply a $\boldsymbol{\beta}$*-KMS state*. To rule out possible phase transitions, we assume that for any given $\boldsymbol{\beta}$ there is a unique gauge-invariant $\boldsymbol{\beta}$-KMS state $\omega_{\boldsymbol{\beta}}$ on $\mathcal{A}(\mathbb{M})$. This assumption also implies that $\omega_{\boldsymbol{\beta}}$ is invariant under spacetime translations. Furthermore we point out that $\boldsymbol{\beta}$-KMS states are quasifree states and fulfill the analytic microlocal spectrum condition [26], in particular they are analytic Hadamard states.

It has been shown in [5] that the correlation functions

$$F_{A,B}(x) = \omega_{\boldsymbol{\beta}}(A\tau_{(1,x)}(B)),\ x \in \mathbb{R}^4$$

of $\boldsymbol{\beta}$-KMS states $\omega_{\boldsymbol{\beta}}$ on $\mathcal{A}(\mathbb{M})$ have in fact stronger analyticity properties than those implied by the KMS condition. These analyticity properties can be seen as a remnant of the relativistic spectrum condition in the case of a thermal equilibrium state.

Definition 1.2 A state $\omega_{\boldsymbol{\beta}}$ on $\mathcal{A}(\mathbb{M})$ satisfies the *relativistic KMS condition* at inverse temperature $\beta > 0$ iff there exists some $e_\beta \in V_+^1$, such that for any $A, B \in \mathcal{A}(\mathbb{M})$ there exists a function $F_{A,B}$ which is defined and holomorphic in the tube $\mathcal{T}_{\beta e_\beta} = \{z \in \mathbb{C}^4 : \Im z \in V_+ \cap (\beta e_\beta + V_-)\}$, where $V_- = -V_+$, and continuous at the boundary sets $\Im z = 0$ and $\Im z = \beta e_\beta$ with

$$F_{A,B}(x) = \omega_{\boldsymbol{\beta}}(A\tau_{(1,x)}(B)), \tag{9}$$

$$F_{A,B}(x + i\beta e_\beta) = \omega_{\boldsymbol{\beta}}(\tau_{(1,x)}(B)A), \quad x \in \mathbb{R}^4. \tag{10}$$

2 The LTE Condition of Buchholz, Ojima and Roos

The first key step in the analysis of Buchholz, Ojima and Roos in [10] is the construction of spaces $\mathcal{Q}_q$ of idealized observables (density-like quantities) located at $q \in \mathbb{M}$. Those observables are well-defined as quadratic forms and their expectation values can be calculated in all states with an appropriate high-energy behaviour. From the spaces $\mathcal{Q}_q$ one then selects subspaces $\mathcal{S}_q \subset \mathcal{Q}_q$ of local thermal observables $s(q)$. The thermal interpretation of these observables is justified by evaluating them in thermal reference states. The set of these reference states is denoted by $\mathcal{C}_B$ and consists of mixtures of KMS states $\omega_{\boldsymbol{\beta}}$, with $\boldsymbol{\beta}$ contained in some compact subset $B \subset V_+$. A generic state $\omega_B \in \mathcal{C}_B$ is represented in the form

$$\omega_B(A) = \int_B \mathrm{d}\mu(\boldsymbol{\beta})\omega_{\boldsymbol{\beta}}(A), \quad A \in \mathcal{A}(\mathbb{M}), \tag{11}$$

where μ is a positive normalized measure on V_+, with support contained in B.

The connection between the local thermal observables from the spaces $\mathcal{S}_q$ and the macroscopic thermal properties of a reference state is provided as follows: As discussed explicitly in [7], the local observables $s(q)$ yield the same information on the thermal properties of the reference states as certain macroscopic observables $\mathfrak{S}$, namely for certain sequences $f_n \in \mathcal{D}(\mathbb{R}^4)$ with $f_n \nearrow 1_{\mathbb{R}^4}$ the limit

$$\mathfrak{S} = \lim_{n\to\infty} s(f_n) \tag{12}$$

exists in all thermal reference states and defines a macroscopic (central) observable, i.e. $\mathfrak{S}$ is commuting with any element $A \in \mathcal{A}$ as well as with the spacetime translations $\tau_{(1,a)}$, $a \in \mathbb{R}^4$. One assumes that all macroscopic intensive thermal parameters of a $\boldsymbol{\beta}$-KMS state are given by maps $\boldsymbol{\beta} \mapsto \mathfrak{S}(\boldsymbol{\beta})$ which are called *thermal functions*. For any $s(q) \in \mathcal{S}_q$ we can define such functions by

$$\boldsymbol{\beta} \mapsto \mathfrak{S}(\boldsymbol{\beta}) := \omega_{\boldsymbol{\beta}}(s(q)), \tag{13}$$

which are Lorentz tensors with the tensorial character depending on $s(q)$. Furthermore, as a consequence of spacetime translation invariance of the states $\omega_{\boldsymbol{\beta}}$, they do not depend on the specific choice of the point $q \in \mathbb{M}$. The thermal functions yield the central decomposition of the macroscopic observables $\mathfrak{S}$ [7]. Thus, we can identify $\mathfrak{S}$ with the respective thermal function $\mathfrak{S}(\boldsymbol{\beta})$ and the states ω_B can be lifted to the space of macroscopic observables via

$$\omega_B(\mathfrak{S})(q) := \omega_B(s(q)), \quad s(q) \in S_q. \tag{14}$$

In the present model the spaces of thermal observables are defined as the spaces $\mathcal{S}_q^n$, spanned by the so-called *balanced derivatives of the Wick square up to order n*. Those are defined as

$$\begin{aligned} &\eth_{\mu_1\dots\mu_n} : \phi^2 : (q) := \\ &\quad \lim_{\xi\to 0} \partial_{\xi^{\mu 1}} \dots \partial_{\xi^{\mu_n}} \left[\phi(q+\xi)\phi(q-\xi) - \omega_{\text{vac}}(\phi(q+\xi)\phi(q-\xi)) \cdot \mathbb{1}\right], \end{aligned} \tag{15}$$

where ω_{vac} is the unique vacuum state on $\mathcal{A}(\mathbb{M})$ and the limit is taken along spacelike directions ξ. Of particular interest is the space $\mathcal{S}_q^2$ which contains (besides the unit $\mathbb{1}$) two thermal observables which play a prominent role. The first one is $:\phi:^2 (q)$, the *Wick square* of ϕ at the point $q \in \mathbb{M}$, which is usually regarded as corresponding to a point-like "thermometer observable" $\Theta(q)$. This is due to the fact

that its evaluation in a $\boldsymbol{\beta}$-KMS state yields for the Klein-Gordon field with $m = 0$[1]:

$$\Theta(\boldsymbol{\beta}) := \omega_{\boldsymbol{\beta}}(:\phi^2:(q)) = \frac{1}{12\beta^2} = \frac{k_B^2}{12}T^2. \tag{16}$$

The other thermal observable contained in $\mathcal{S}_q^2$ is $\eth_{\mu\nu} : \phi^2 : (q)$, the second balanced derivative of $: \phi^2 : (q)$. It is of special interest since its expectation values in a $\boldsymbol{\beta}$-KMS state $\omega_{\boldsymbol{\beta}}$ are (up to a constant) equal to the expectation values of the thermal stress-energy tensor [10]:

$$E_{\mu\nu}(\boldsymbol{\beta}) := -\frac{1}{4}\omega_{\boldsymbol{\beta}}(\eth_{\mu\nu} : \phi^2 : (q)) = \frac{\pi^2}{90}\left(4\boldsymbol{\beta}_\mu\boldsymbol{\beta}_\nu - \boldsymbol{\beta}^2\eta_{\mu\nu}\right)(\boldsymbol{\beta}^2)^{-3}. \tag{17}$$

For the Klein-Gordon field with $m = 0$ an easy computation yields [10]:

$$\mathfrak{S}^{(n)}(\boldsymbol{\beta}) := \omega_{\boldsymbol{\beta}}(\eth_{\mu 1\cdots\mu_n} : \phi^2 : (q)) = c_n \partial^{\boldsymbol{\beta}}_{\mu 1} \ldots \partial^{\boldsymbol{\beta}}_{\mu_n} \left(\boldsymbol{\beta}^2\right)^{-1}. \tag{18}$$

This makes clear that the thermal functions $\mathfrak{S}^{(n)}(\boldsymbol{\beta})$ can be constructed completely out of $\boldsymbol{\beta}$.[2] Thus they can be viewed as thermal functions corresponding to the micro-observables $s(q)$. Furthermore, due to the invariance of $\omega_{\boldsymbol{\beta}}$ under spacetime translations, they are independent of q. Note, that for odd n the thermal functions are equal to 0.

The definition of local thermal equilibrium in the sense of [7, 10] can now be stated for the quantized Klein-Gordon field[3] as follows:

Definition 2.1 Let $\mathcal{O} \subset \mathbb{M}$ and ω a Hadamard state on $\mathcal{A}(\mathbb{M})$.

(1) We say that ω is a *local thermal equilibrium state of order N in $\mathcal{O}$ with sharp inverse temperature vector field* $\boldsymbol{\beta}(\mathcal{O})$, or $[\boldsymbol{\beta}(\mathcal{O}), N]$-*LTE state* for short, iff there exists a continuous (resp. smooth, if $\mathcal{O}$ is open) map $\boldsymbol{\beta} : \mathcal{O} \to V_+$ for any $q \in \mathcal{O}$ it holds

$$\omega(s(q)) = \omega_{\boldsymbol{\beta}(q)}(s(q)) \quad \forall s(q) \in \mathcal{S}_q^n,\ n \leq N, \tag{19}$$

where $\omega_{\boldsymbol{\beta}(q)}$ is the unique extremal $\boldsymbol{\beta}(q)$-KMS state on $\mathcal{A}(\mathbb{M})$

(2) We say that ω is a *local thermal equilibrium state of order N in $\mathcal{O}$ with mixed temperature distribution* μ, or $[\mu, \mathcal{O}, N]$-*LTE state* for short, iff there exists a

[1] In the massive case the expression $\omega_{\boldsymbol{\beta}}(:\phi^2:(q))$ yields a slightly more complicated but still monotonously decreasing function of β.

[2] This is also true in the massive case. Here, the thermal functions are given by a more involved expression which is analytic in $\boldsymbol{\beta}$ [17].

[3] In [10] a definition has been given which is valid for more general quantum fields ϕ, also including interacting ones.

function $\mu : q \mapsto \mu_q, q \in \mathcal{O}$, where each μ_q is a probability measure with support in some compact $B(q) \subset V_+$, and for any $q \in \mathcal{O}$

$$\omega(s(q)) = \omega_{B(q)}(s(q)), \quad \forall s(q) \in S^n_q,\ n \leq N, \tag{20}$$

where the states $\omega_{B(q)}, q \in \mathcal{O}$ are defined by

$$\omega_{B(q)}(A) = \int_{B(q)} d\mu_q(\boldsymbol{\beta})\omega_{\boldsymbol{\beta}}(A), \quad A \in \mathcal{A}(\mathbb{M}). \tag{21}$$

We say that ω is a $[\mu, \mathcal{O}]$-LTE state iff (20) holds for all $n \in \mathbb{N}$.

It is obvious from this definition that any $\boldsymbol{\beta}$-KMS state $\omega_{\boldsymbol{\beta}}$ is a $\boldsymbol{\beta}(\mathbb{M})$-LTE state with constant inverse temperature vector field given by $\boldsymbol{\beta}(q) \equiv \boldsymbol{\beta}$. Although this should be the case for consistency reasons the noteworthy feature of the above definition lies in the possibility of a *varying* inverse temperature vector field $\boldsymbol{\beta}$, so an LTE state can have varying inverse temperature β_q (resp. inverse temperature distribution μ_q) as well as varying rest frame at each $q \in \mathcal{O}$.

It is known from special relativistic thermodynamics that all relevant macroscopic thermal parameters, in particular the entropy current density, for a (local) equilibrium state can be constructed once the components of $E_{\mu\nu}$ are known [12, Chapter 4]. This means that in order to gain knowledge about the coarse macroscopic properties of (local) equilibrium states it is sufficient to analyze them by means of the subset S^2_q of all thermal observables. For increasing n the spaces $\mathcal{S}^n_q$ contain more and more elements, i.e. the higher balanced derivatives of $:\phi^2:(q)$. Thus, the $[\boldsymbol{\beta}(\mathcal{O}), N]$-LTE condition introduces a hierarchy among the local equilibrium states in the following sense: If we successively increase the order N in this condition we obtain an increasingly finer resolution of the thermal properties of this state. For finite N we obtain a measure of the deviation of the state ω from complete local thermal equilibrium (which would amount to a $\boldsymbol{\beta}(\mathcal{O})$-LTE state).

An example of a $\boldsymbol{\beta}(\mathcal{O})$-LTE state on $\mathcal{A}(\mathbb{M})$ (massless case), with $\mathcal{O} = V_+$, has been given in [10]. It is a quasifree state ω_{hb} on $\mathcal{A}(\mathbb{M})$, the so-called *hot bang state* defined via

$$\omega^{\mathrm{hb}}_2(x, y) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^4} d^4p\, \frac{\varepsilon(p_0)\delta(p^2)}{1 - e^{-\gamma(x+y)p}} e^{-ip(x-y)}, \qquad x + y \in V_+, \tag{22}$$

where $\gamma > 0$ is a real parameter. One finds immediately that for all $q \in V_+$

$$\omega_{\mathrm{hb}}(\eth_{\mu 1 \ldots \mu_n} : \phi^2 : (q)) = \omega_{\boldsymbol{\beta}(q)}(\eth_{\mu 1 \ldots \mu_n} : \phi^2 : (q)), \tag{23}$$

where $\omega_{\boldsymbol{\beta}(q)}$ is the unique extremal $\boldsymbol{\beta}(q)$-KMS state with $\boldsymbol{\beta}(q) = 2\gamma q, q \in V_+$. Thus, the state ω_{hb} in fact is a $\boldsymbol{\beta}(V_+)$-LTE state in the sense of Definition 2.1. It describes the spacetime evolution of a "heat explosion" with infinite temperature at the tip of the forward lightcone V_+ which justifies the name hot bang state. For a

more thorough discussion of the properties of ω_{hb} we refer to the article by Buchholz [7]. Below we will see that such a state is in fact the generic example of an infinite-order and sharp-temperature LTE state of the massless Klein-Gordon field.

3 A Local Version of the KMS Condition

The LTE condition of [10] is based on the heuristic assumption that one should be able to obtain information about the (macroscopic) thermal properties of near-to-equilibrium states by comparing them pointwise to thermal reference states (KMS states or mixtures of such) by means of localized thermal observables. In the present model those observables were modelled by the Wick square $:\phi^2:(q)$ and its balanced derivatives. This choice has been largely motivated by the fact that the expectation value of the Wick square in equilibrium is proportional to the square of the equilibrium temperature (i.e. temperature in the sense of the 0th law of thermodynamics). It would clearly be desirable to give further arguments for the special choice of the thermal observables in the free field case. A physical motivation, based on the investigation of the behaviour of moving detectors modelled by quantum mechanical two-level systems (Unruh detectors), has been given in [20]. On the mathematical side, in view of the definition of the balanced derivatives of the Wick square, Eq. (15), one should be able to encode the thermal properties of an LTE state ω on $\mathcal{A}(\mathbb{M})$ directly on the level of the two-point functions ω_2. This assumption is further strengthened by observing that the correlation functions $\omega_2^{\boldsymbol{\beta}}(q \mp \xi, q \pm \xi)$ for a $\boldsymbol{\beta}$-KMS state are completely determined by the expectation values $\omega_{\boldsymbol{\beta}}(\eth_{\mu_1 \cdots \mu_n} :\phi^2:(q))$ for all $n \in \mathbb{N}$, as discussed in [10]. In the following we will discuss a recent proposal by Gransee, Pinamonti and Verch [14] for characterizing LTE states by properties of their two-point function ω_2 which are similar to the KMS condition. It will turn out that under reasonable additional analyticity requirements this characterization yields the class of $[\boldsymbol{\beta}(\mathcal{O}), N]$-LTE states, which were introduced in the previous section.

A first observation in [14] is, that for any Hadamard state ω on $\mathcal{A}(\mathbb{M})$ and any $q \in \mathbb{M}$ the "function" $\mathfrak{w}_q$, given by

$$\mathfrak{w}_q(\xi) := \omega_2(q - \xi, q + \xi), \quad \xi \in \mathbb{R}^4, \tag{24}$$

can be meaningfully defined as a distribution in $\mathcal{S}'(\mathbb{R}^4)$. In particular, for any timelike future-pointing unit vector $e \in V_+^1$ the "function" $\mathfrak{u}_{q,e}$, defined by

$$\mathfrak{u}_{q,e}(t) := \omega_2(q - te, q + te), \quad t \in \mathbb{R}, \tag{25}$$

is well-defined as a distribution in $\mathcal{S}'(\mathbb{R})$. If $\omega_{\boldsymbol{\beta}}$ is a $\boldsymbol{\beta}$-KMS state on $\mathcal{A}(\mathbb{M})$ it follows from the spacetime translation invariance of such states that the distribution $\mathfrak{u}_{\boldsymbol{\beta}}$, defined by

$$\mathfrak{u}_{\boldsymbol{\beta}}(t) := \omega_2^{\boldsymbol{\beta}}\left(q - te_\beta, q + te_\beta\right) \tag{26}$$

is independent of the choice of the point $q \in \mathbb{M}$. The role of the parameter t is enlightened by the following observation: *If $\omega_{\boldsymbol{\beta}}$ is a $\boldsymbol{\beta}$-KMS state on $\mathcal{A}(\mathbb{M})$, then for arbitrary but fixed $q \in \mathbb{M}$ there is a complex function $f_{\boldsymbol{\beta}}$, holomorphic on the strip S_β, with (distributional) boundary values*

$$f_{\boldsymbol{\beta}}(t) = \omega_2^{\boldsymbol{\beta}}\left(q - te_\beta, q + te_\beta\right) \quad \text{and} \quad f_{\boldsymbol{\beta}}(t + i\beta) = \omega_2^{\boldsymbol{\beta}}\left(q + te_\beta, q - te_\beta\right). \tag{27}$$

This is to be seen as a remnant of the KMS condition, in which the parameter t plays the same role as the parameter of the one-parametric group of time evolution on $\mathcal{A}(\mathbb{M})$, and where the boundary value conditions (6) and (7) are replaced by the weaker property (27) above. However, the above properties are surely not sufficient to imply the $\boldsymbol{\beta}$-KMS condition. The main point is that these properties are valid with respect to an a priori fixed point $q \in \mathbb{M}$ and therefore do not tell us anything about spacetime translation invariance of the state $\omega_{\boldsymbol{\beta}}$. Furthermore, the knowledge of the distribution $\mathfrak{u}_q \in \mathcal{S}'(\mathbb{R})$ (which arises as the restriction of the distribution $\mathfrak{w}_q \in \mathcal{S}'(\mathbb{R}^4)$ to the set $\{\xi \in \mathbb{R}^4 : \xi = te_q, t \in \mathbb{R}\}$) does not completely determine the correlation functions $\omega(q \mp \xi, q \pm \xi)$ but only their restrictions to timelike arguments ξ. However, if one makes the additional assumption that the state ω fulfills the analytic Hadamard condition (5), one observes [14]:

Observation *An analytic Hadamard state ω fulfills the $\boldsymbol{\beta}(q)$-LTE condition if and only if there exists a $\boldsymbol{\beta}(q) \in V_+$ such that*

$$\mathfrak{w}_q(\xi) = \mathfrak{w}_{\boldsymbol{\beta}(q)}(\xi) = \frac{1}{(2\pi)^3}\int d^4p \frac{\varepsilon(p_0)\delta(p^2 - m^2)}{1 - e^{-\boldsymbol{\beta}(q)p}} e^{-ip\xi}, \tag{28}$$

which is to be understood in the sense of distributions.

This shows that the $\boldsymbol{\beta}(q)$-LTE condition together with the analytic Hadamard condition is sufficient to determine the correlation functions $\omega(q \mp \xi, q \pm \xi)$ completely. As mentioned above, the respective correlation functions for the comparison equilibrium state $\omega_{\boldsymbol{\beta}(q)}$ are completely fixed by the expectation values $\omega_{\boldsymbol{\beta}(q)}(\mathfrak{d}_{\mu_1 \ldots \mu_n} : \phi^2 : (q))$ for any $q \in \mathcal{O}$. This provides an additional justification for the use of the balanced derivatives as the thermal observables in the present model. Analyzing the analyticity properties of the correlation functions $\mathfrak{w}_{\boldsymbol{\beta}(q)}(\xi)$, the above observation is used in [14] to relax the KMS condition as follows:

Definition 3.1 Let $q \in \mathbb{M}$ and ω be an analytic Hadamard state on $\mathcal{A}(\mathbb{M})$. We say that ω fulfills the *local KMS condition at q with respect to $\boldsymbol{\beta}(q)$*, or *$\boldsymbol{\beta}(q)$-LKMS*

condition for short, iff there exists a $\boldsymbol{\beta}(q) \in V_+$ and a complex function F_q with the following properties:

(i) F_q is defined and holomorphic in the (flat) tube

$$\mathcal{T}_q = \{z \in \mathbb{C}^4 : \Im z = \sigma e_q, 0 < \sigma < \beta_q\}. \tag{29}$$

(ii) For all compact $K \subset (0, \beta)$ there exist constants $C_K > 0$ and $N_K \in \mathbb{N}_0$ such that

$$\left|F_q(\xi + i\sigma e_q)\right| \leq C_K(1 + \left|\xi + i\sigma e_q\right|)^{N_K}, \quad \xi \in \mathbb{R}^4, \sigma \in K. \tag{30}$$

(iii) We have in the sense of distributions:

$$F_q(\xi + i\sigma e_q) \xrightarrow[\sigma \to 0^+]{} \mathfrak{w}_q(\xi), \tag{31}$$

$$F_q(\xi + i(\beta_q - \eta)e_q) \xrightarrow[\eta \to 0^+]{} \mathfrak{w}_q(-\xi), \tag{32}$$

(iv) We have the following clustering property:

$$\mathfrak{w}_q(te_q) \xrightarrow[|t| \to \infty]{} 0. \tag{33}$$

Let $\mathcal{O}$ be a spacetime region. We say that ω fulfills the $\boldsymbol{\beta}(\mathcal{O})$-*LKMS condition*, iff there exists a continuous (resp. smooth, if $\mathcal{O}$ is open) map $\boldsymbol{\beta} : \mathcal{O} \to B \subset V_+$ such that ω fulfills the $\boldsymbol{\beta}(q)$-LKMS condition for all $q \in \mathcal{O}$.

Any $\boldsymbol{\beta}$-KMS state $\omega_{\boldsymbol{\beta}}$ is a $\boldsymbol{\beta}(\mathcal{O})$-LKMS state with $\mathcal{O} = \mathbb{M}$, where $\beta_q \equiv \beta$ and $e_q \equiv e_{\boldsymbol{\beta}}$ are constant throughout Minkowski spacetime. However, the natural question arises if there are other examples of nontrivial LKMS states. We first note that the $\boldsymbol{\beta}(q)$-LKMS condition can be shown [14] to have an equivalent momentum-space formulation: *A state ω on $\mathcal{A}(\mathbb{M})$ fulfills the $\boldsymbol{\beta}(q)$-LKMS condition if and only if there exists a $\boldsymbol{\beta}(q) = \beta_q e_q \in V_+$, such that in the sense of distributions*

$$\hat{\mathfrak{w}}_q(p) = e^{\boldsymbol{\beta}(q)p}\hat{\mathfrak{w}}_q(-p), \tag{34}$$

and the cluster property (33) *holds.*

The relation (34) can be seen as a remnant of the $\boldsymbol{\beta}$-KMS condition in momentum space [6]. With the definition (22) of the hot-bang state ω_{hb} one sees that the latter is an example of a $\boldsymbol{\beta}(\mathcal{O})$-LKMS state with $\mathcal{O} = V_+$ and $\boldsymbol{\beta}(q) = 2\gamma q$. Thus, the local KMS condition appears as a non-trivial generalization of the KMS condition. More generally, relations (33) and (34) yield

$$\hat{\mathfrak{w}}_q(p) = \frac{1}{2\pi} \frac{\varepsilon(p_0)\delta(p^2 - m^2)}{1 - e^{-\boldsymbol{\beta}(q)p}} = \hat{\mathfrak{w}}_{\boldsymbol{\beta}(q)}(p) \tag{35}$$

This shows that the $\boldsymbol{\beta}(q)$-LKMS condition (in position or in momentum space) is sufficient to completely determine the correlation functions $\mathfrak{w}_q(\xi)$. In consequence, this proves:

Theorem 3.2 *Let $q \in \mathbb{M}$ and ω an analytic Hadamard state on $\mathcal{A}(\mathbb{M})$. Then the following are equivalent:*

(i) ω is a $\boldsymbol{\beta}(q)$-LTE state.
(ii) ω fulfills the $\boldsymbol{\beta}(q)$-LKMS condition.

LKMS and finite-order LTE states For LTE states of finite order (in the sense of Definition 2.1) it seems to be clear that the relation (28) will not be valid exactly, but that a similar relation might hold. Informally, in view of the definition of the balanced derivatives (15), one would expect the following to hold: *The directional derivatives with respect to ξ of the correlation functions $\omega(q \mp \xi, q \pm \xi)$ at the point $\xi = 0$ coincide with those of the respective correlation functions of a comparison equilibrium state $\omega_{\boldsymbol{\beta}(q)}$, up to order N.*

Of course, from a mathematical point of view, this statement is meaningless, because the correlation functions are distributions in $\mathcal{S}'(\mathbb{R}^4)$ and it is not clear what is meant by "the directional derivatives of $\omega(q \mp \xi, q \pm \xi)$ at the point $\xi = 0$". Nevertheless, one has a mathematically well-defined version of the above informal statement [14]:

Observation *Let $q \in \mathbb{M}$. An analytic Hadamard state ω on $\mathcal{A}(\mathbb{M})$ fulfills the $[\boldsymbol{\beta}(q), N]$-LTE condition if and only if there exists a $\boldsymbol{\beta}(q) \in V_+$ such that*

$$[\partial_{\underline{\alpha}}(\mathfrak{w}_{\boldsymbol{\beta}(q)} - \mathfrak{w}_q)](0) = 0 \quad \forall \underline{\alpha} \in \{\underline{\alpha} \in \mathbb{N}_0^4 : |\underline{\alpha}| \leq N\}, \tag{36}$$

where $\mathfrak{w}_{\boldsymbol{\beta}(q)}(\xi) = \omega_2^{\boldsymbol{\beta}(q)}(q - \xi, q + \xi)$ for the unique $\boldsymbol{\beta}(q)$-KMS state $\omega_{\boldsymbol{\beta}(q)}$.

This observation can be used to further generalize the $\boldsymbol{\beta}(q)$-LKMS condition:

Definition 3.3 Let $q \in \mathbb{M}$ and $N \in \mathbb{N}$. An analytic Hadamard state ω on $\mathcal{A}(\mathbb{M})$ is said to fulfill the $[\boldsymbol{\beta}(q), N]$-*LKMS condition* iff there exists a $\boldsymbol{\beta}(q) \in V_+$ such that there is a complex function F_q with the following properties:

(i) F_q is defined and holomorphic in the (flat) tube

$$\mathcal{T}_q = \{z \in \mathbb{C}^4 : \Im z = \sigma e_q, 0 < \sigma < \beta_q\}. \tag{37}$$

(ii) For all compact $K \subset (0, \beta_q)$ there exist constants $N_K \in \mathbb{N}$ and $C_K > 0$ such that

$$\left|F_q(\xi + i\sigma e_q)\right| \leq C_K(1 + \left|\xi + i\sigma e_q\right|)^{N_K}, \qquad \forall\, \sigma \in K. \tag{38}$$

(iii) There exists a symmetric $R_q \in \mathcal{S}'(\mathbb{R}^4)$ with $\mathrm{WF}_A(R_q) = \emptyset$ and

$$[\partial^{\underline{\alpha}} R_q(0)] = 0 \quad \forall \underline{a} \in \{\underline{\alpha} \in \mathbb{N}_0^4 : |\underline{a}| \leq N\}, \tag{39}$$

$$(\mathfrak{w}_q + R_q)(te_q) \xrightarrow[|t|\to\infty]{} 0\,, \tag{40}$$

such that in the sense of distributions

$$F_q(\xi + i\sigma e_q) \xrightarrow[\sigma\to 0^+]{} (\mathfrak{w}_q + R_q)(\xi), \tag{41}$$

$$F_q(\xi + i(\beta_q - \eta)e_q) \xrightarrow[\eta\to 0^+]{} (\mathfrak{w}_q + R_q)(-\xi). \tag{42}$$

(iv) We have the following cluster property:

$$(\mathfrak{w}_q + R_q)(te_q) \xrightarrow[|t|\to\infty]{} 0. \tag{43}$$

This definition can also be generalized to open regions $\mathcal{O}$ of Minkowski spacetime. An analogous analysis as for the $\boldsymbol{\beta}(q)$-LKMS condition shows that the $[\boldsymbol{\beta}(q), N]$-LKMS condition is sufficient to determine the correlation functions $\omega(q \mp \xi, q \pm \xi)$, similar to (28), but only up to some real-analytic "rest term" $R_q : \mathbb{R}^4 \to \mathbb{R}^4$. Without going into details, we want to state that this implies the following result:

Theorem 3.4 *Let $q \in \mathbb{M}$ and ω an analytic Hadamard state on $\mathcal{A}(\mathbb{M})$. Then the following are equivalent:*

(i) ω is a $[\boldsymbol{\beta}(q), N]$-LTE state.
(ii) ω fulfills the $[\boldsymbol{\beta}(q), N]$-LKMS condition.
(iii) There exists a $\boldsymbol{\beta}(q) = \beta_q e_q \in V_+$ and a symmetric $\hat{R}_q \in \mathcal{S}'(\mathbb{R}^4)$ with

$$\mathcal{F}[p^{\underline{\alpha}}\hat{R}_q(p)](0) = 0 \quad \forall \underline{\alpha} \in \{\underline{\alpha} \in \mathbb{N}_0^4 : |\underline{\alpha}| \leq N\}, \tag{44}$$

such that the cluster property (43) holds and we have in the sense of distributions:

$$e^{\boldsymbol{\beta}(q)p}(\hat{\mathfrak{w}}_q + \hat{R}_q)(-p) = (\hat{\mathfrak{w}}_q + \hat{R}_q)(p). \tag{45}$$

For a proof of Theorem 3.4 we again refer to [14].

Constraints from the Klein-Gordon equation A further interesting question is the following: Given a $[\boldsymbol{\beta}(\mathcal{O}), N]$-LKMS state for some (open) subset $\mathcal{O}$, is the form of the map $\boldsymbol{\beta} : \mathcal{O} \to V_+$ completely arbitrary? Surely, this is not the case if the comparison equilibrium states $\omega_{\boldsymbol{\beta}(q)}$ ought to fulfill the (relativistic) KMS condition. It turns out (cf. also [7, 17]) that the equations of motion for the field ϕ imply dynamical constraints on the correlation functions $\mathfrak{w}_q(\xi)$ which give restrictions on the map $\boldsymbol{\beta}$. For the case of the massless Klein-Gordon field on can prove the following [14]:

Proposition 3.5 *Let $\omega \subset \mathbb{M}$ be an analytic Hadamard state on $\mathcal{A}(\mathbb{M})$ which fulfills the $\boldsymbol{\beta}(\mathcal{O})$-LKMS condition. Then there exists $\boldsymbol{b} \in \mathbb{R}^4$ such that $\mathcal{O} \subset \{V_+ - \boldsymbol{b}\}$ (resp. $\mathcal{O} \subset \{-V_+ - \boldsymbol{b}\}$) and*

$$\boldsymbol{\beta}^\mu(q) = c_\omega q^\mu + \boldsymbol{b}^\mu \quad \forall q \in \mathcal{O}, \tag{46}$$

where $c_\omega > 0$ (resp. $c_\omega < 0$) is a state-dependent constant.

If we exclude the somewhat unphysical case $c_\omega < 0$ this makes clear that the hot-bang state ω_{hb}, defined by (22), is the generic example of a $\boldsymbol{\beta}(\mathcal{O})$-LKMS state. Namely, the analytic Hadamard condition on a $\boldsymbol{\beta}(\mathcal{O})$-LKMS state ω implies that $\mathfrak{w}_q = \mathfrak{w}_{\boldsymbol{\beta}(q)}$ for all $q \in \{V_+ - \boldsymbol{b}\}$ and, in consequence, that ω fulfills the $\boldsymbol{\beta}(\{V_+ - \boldsymbol{b}\})$-LKMS condition, with

$$\boldsymbol{\beta}^\mu(q) = c_\omega q^\mu + \boldsymbol{b}^\mu \quad \forall q \in \{V_+ - b\}. \tag{47}$$

The hot-bang state then corresponds to $\boldsymbol{b} = 0$ and any other $\boldsymbol{\beta}(\mathcal{O})$-LKMS state arises from ω_{hb} by $\omega = \omega_{\mathrm{hb}} \circ \tau_{(1,-\boldsymbol{b})}, \quad \boldsymbol{b} \in \mathbb{R}^4$.

For the massive Klein-Gordon field the situation is even more restrictive: In this case it turns out that for $\omega \subset \mathbb{M}$ the only states which can fulfill the $\boldsymbol{\beta}(\mathcal{O})$-LKMS condition are the states for which $\boldsymbol{\beta}(q) = \text{const.}$ for all $q \in \mathcal{O}$. The analytic Hadamard condition on $\mathcal{O}$ then implies that ω has to be the unique $\boldsymbol{\beta}$-KMS state $\omega_{\boldsymbol{\beta}}$ on $\mathcal{A}(\mathbb{M})$. Thus, there are no nontrivial infinite-order LTE states of the massive Klein-Gordon field.

LTE states with mixed temperature The above discussion implies that states of the massive Klein-Gordon field which are thermal in a subset $\mathcal{O} \subset \mathbb{M}$ always have to be mixed-temperature LTE states in the sense of Definition 2.1, characterized at each $q \in \mathcal{O}$ by some probability measure μ_q. In [17] Hübener succeeded in constructing a specific example of a $[\mu_q, \mathcal{O}]$-LTE state. Apart from this, one has the following general existence result [10]:

Proposition 3.6 *Let $q \in \mathbb{M}$. For every finite-dimensional subspace S_q^N of all thermal observables and any compact $B_q \subset V_+$ there exists a probability measure μ_q, with support contained in B_q, and states ω on $\mathcal{A}(\mathbb{M})$ which are $[\mu_q, N]$-thermal.*

This result has been generalized by Solveen [23] as follows:

Proposition 3.7 *Let $\mathcal{O}$ be a compact region of Minkowski spacetime. For every finite-dimensional subspace S_q^N of all thermal observables there exists a map $\mu : q \mapsto \mu_q, q \in \mathcal{O}$, where μ_q is a probability measure compactly supported in V_+, and states ω on $\mathcal{A}(\mathbb{M})$ which are $[\mu(\mathcal{O}), N]$-thermal.*

In view of these existence results, it seems to be desirable to give an intrinsic characterization of such states similar to the LKMS condition. Similar to the case of sharp-temperature LTE states one observes the following [14]:

Observation *Let $q \in \mathbb{M}$. An analytic Hadamard state ω on $\mathcal{A}(\mathbb{M})$ fulfills the $[\mu, \{q\}, N]$-LTE condition if and only if there exists a probability measure μ_q with*

support in some compact $B(q) \subset V_+$*, such that*

$$[\partial_{\underline{\alpha}}(\mathfrak{w}_{B(q)} - \mathfrak{w}_q)](0) = 0 \quad \forall \underline{\alpha} \in \{\underline{\alpha} \in \mathbb{N}_0^4 : |\underline{\alpha}| \leq N\}, \tag{48}$$

where $\mathfrak{w}_{B(q)}(\xi) = \int_{B(q)} d\mu_q(\boldsymbol{\beta})\mathfrak{w}_\beta(\xi)$.

Unfortunately, one immediately obtains that, although the distribution $\mathfrak{w}_{B(q)}$ can be extended to a holomorphic function on a subset of $\mathbb{C}^4$, it does not have periodicity properties in the imaginary space-time variable, since the state $\omega_{B(q)}$ does not fulfill the KMS condition with respect to some $\boldsymbol{\beta} \in V_+$. However, there might be the possibility to characterize such states by remnants of the so-called *auto-correlation inequalities*, which yield another (equivalent) characterization of equilibrium states in algebraic quantum statistical mechanics (see e.g. [4, Thm. 5.3.15 and Thm. 5.3.17]). This problem is currently under investigation.

4 Summary and Outlook

In this article we reviewed some aspects of local thermal equilibrium states in relativistic quantum field theory. The necessity to introduce such states arises since one would like to describe the macroscopic properties of states in quantum field theory which are not global equilibrium (KMS) states, but locally still possess well-defined thermal parameters, like temperature and thermal stress-energy. For the characterization of LTE states of the quantized Klein-Gordon field on Minkowski spacetime one has in principle two options. One could describe these states in operational way, as it has been done in [10], which results in an (extrinsic) LTE condition. On the other hand, one could aim at a more intrinsic characterization, based on properties of correlation functions, in the spirit of the KMS condition. Such a generalized KMS condition, called local KMS condition, has been introduced in [14], and it turns out that, under additional (physically motivated) analyticity assumptions on the two-point function, both approaches yield the same class of non-equilibrium states of the quantized Klein-Gordon field on Minkowski spacetime.

Finally, we want to mention that the concept of LTE states has also been generalized to include quantum fields on a generic curved spacetime [11, 22, 24] and some results concerning the thermal behaviour of quantum fields in cosmological spacetimes of Friedmann-Robertson-Walker type [28] have been established [13, 18, 21]. For an overview and a more in-depth discussion of these results and other results concerning LTE states in quantum field theory, we refer the interested reader to the exhaustive review article by Verch [27] and the references therein. It clearly is a challenging task to try to generalize the results concering the LKMS condition also to situations in which gravity is present, i.e. in which space-time is curved.

Acknowledgements The author wants to thank the organizers of the conference "Quantum Mathematical Physics" for their invitation and kind hospitality during his stay in Regensburg. Parts of the work on the LKMS condition have been carried out during a stay at the ESI in Vienna for the conference "Algebraic Quantum Field Theory – Its status and its future" in May 2014. Financial support from the International Max Planck Research School "Mathematics in the Sciences" is gratefully acknowledged.

References

1. H. Araki, *Mathematical Theory of Quantum Fields*. International Series of Monographs on Physics, vol. 101 (Oxford University Press, New York, 2009)
2. M. Benini, C. Dappiaggi, T.-P. Hack, Quantum field theory on curved backgrounds – a primer. Int. J. Mod. Phys. A **28**, 1330023 (2013)
3. H.J. Borchers, On revolutionizing quantum field theory with Tomita's modular theory. J. Math. Phys. **41**, 3604–3673 (2000)
4. O. Bratteli, D.W. Robinson, *Operator Algebras and Quantum Statistical Mechanics 2*, 2nd edn. (Springer, Berlin, 1997)
5. J. Bros, D. Buchholz, Towards a relativistic KMS-condition. Nucl. Phys. **B429**, 291–318 (1994)
6. J. Bros, D. Buchholz, Axiomatic analyticity properties and representations of particles in thermal quantum field theory. Ann. Poincare Phys. Theory **64**, 495–522 (1996)
7. D. Buchholz, On hot bangs and the arrow of time in relativistic quantum field theory. Commun. Math. Phys. **237**, 271–288 (2003)
8. D. Buchholz, P. Junglas, Local properties of equilibrium states and the particle spectrum in quantum field theory. Lett. Math. Phys. **11**, 51 (1986)
9. D. Buchholz, P. Junglas, On the existence of equilibrium states in local quantum field theory. Commun. Math. Phys. **121**, 255–270 (1989)
10. D. Buchholz, I. Ojima, H. Roos, Thermodynamic properties of non-equilibrium states in quantum field theory. Ann. Phys. **297**, 219–242 (2002)
11. D. Buchholz, J. Schlemmer, Local temperature in curved spacetime. Class. Quantum Gravity **24**, F25–F31 (2007)
12. W.G. Dixon, *Special Relativity* (Cambridge University Press, Cambridge/New York, 1978)
13. M. Gransee, *Thermisches Verhalten des quantisierten Skalarfeldes auf Friedmann-Robertson-Walker-Raumzeiten*, Diploma thesis, Universität Leipzig, 2010
14. M. Gransee, N. Pinamonti, R. Verch, *Local Thermal Equilibrium as a Generalization of the KMS-condition* (in preparation)
15. R. Haag, *Local Quantum Physics* (Springer, Berlin/New York, 1992)
16. R. Haag, N.M. Hugenholtz, M. Winnink, On the Equilibrium states in quantum statistical mechanics. Commun. Math. Phys. **5**, 215–236 (1967)
17. R. Hübener, *Lokale Gleichgewichtszustände massiver Bosonen*, Diploma thesis, Universität Göttingen, 2005
18. A. Knospe, *Lokales thermales Gleichgewicht und Quanten-Energie-Ungleichungen für Dirac-Felder auf gekrümmten Raumzeiten*, Diploma thesis, Universität Leipzig, 2010
19. H. Sahlmann, R. Verch, Microlocal spectrum condition and Hadamard form for vector valued quantum fields in curved space-time. Rev. Math. Phys. **13**, 1203–1246 (2001)
20. J. Schlemmer, *Local Thermal Equilibrium States and Unruh Detectors in Quantum Field Theory* (2007). arXiv preprint: hep-th/0702096
21. J. Schlemmer, *Local Thermal Equilibrium on Cosmological Spacetimes*, Ph.D. thesis, Universität Leipzig, 2010
22. J. Schlemmer, R. Verch, Local thermal equilibrium states and quantum energy inequalities. Ann. Henri Poincare **9**, 945–978 (2008)

23. C. Solveen, Local thermal equilibrium in quantum field theory on flat and curved spacetimes. Class. Quantum Gravity **27**, 235002 (2010)
24. C. Solveen, Local thermal equilibrium and kms states in curved spacetime. Class. Quantum Gravity **29**, 245015 (2012)
25. R.F. Streater, A.S. Wightman, *PCT, Spin and Statistics, and All That* (Princeton University Press, Princeton, 2000)
26. A. Strohmaier, R. Verch, M. Wollenberg, Microlocal analysis of quantum fields on curved space-times: analytic wavefront sets and Reeh-Schlieder theorems. J. Math. Phys. **43**, 5514–5530 (2002)
27. R. Verch, Local covariance, renormalization ambiguity, and local thermal equilibrium in cosmology, in *Quantum Field Theory and Gravity*, ed. by F. Finster et al. (Birkhäuser, Basel, 2012), pp. 229–256
28. R.M. Wald, *General Relativity* (The University of Chicago Press, Chicago, 1984)

Categorical Methods in Quantum Field Theory

Frédéric Paugam

Contents

Abstract We give an introduction to the categorical methods used in the book "Towards the Mathematics of Quantum Field Theory" (Paugam F, Towards the mathematics of quantum field theory. Springer, Cham, 2014), to which we refer for the details of our work and a list of references. The main interest of our approach is that it gives a clear mathematical status to the various "spaces of fields" that appear in the treatment of general classical and quantum gauge theories.

Keywords Covariant field theory • Functor of points • Local and non-local functionals • D-geometry • Differential spaces • Gauge theories

F. Paugam (✉)
Institut de Mathématiques de Jussieu, Université Pierre et Marie Curie, Analyse Algébrique, 5–18 15–25, 4, place de Jussieu, F-75005 Paris, France
e-mail: frederic.paugam@imj-prg.fr

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_7

Mathematics Subject Classification (2010). 81T70, 81T13, 58A03, 58A20, 18G55

1 Pure Yang-Mills and Derived Smooth Spaces

Before giving the basic definitions necessary to understand what derived smooth spaces are, we will explain how they appear in an important and concrete physical example.

Let (M, g) be a metric variety and G a semisimple group, with Killing form

$$\langle \cdot, \cdot \rangle : \mathfrak{g} \times \mathfrak{g} \to \mathbb{R}.$$

The configuration space for the equations of motion is given by the moduli space $\mathrm{BunCon}_G(M)$ whose points are given by pairs (P, A) with:

1. P a principal G-bundle on M,
2. A a principal G-connection on P.

The aim of classical mechanics is to minimize the action functional

$$S(P, A) = \int_M F_A \wedge *F_A \, d\mu_g$$

with some boundary values on a convenient domain. Here, F_A is the connection's curvature form, $*$ is the Hodge star operator associated to the metric g and $d\mu_g$ the Riemannian measure.

We would like to see this action functional as a smooth function on a smooth space $\mathrm{BunCon}_G(M)$. In order to equip this space with a smooth structure, we may first see it as a diffeological space, i.e., a set-valued sheaf on the category $\mathrm{Open}_{\mathcal{C}^\infty}$ of open subspaces of $\mathbb{R}^n$ for varying n.

Recall that the manifold M may itself be seen as such a sheaf

$$\underline{M} : \mathrm{Open}_{\mathcal{C}^\infty}^{op} \to \textsc{Sets}$$

defined by $\underline{M}(U) = \mathrm{Hom}_{\mathcal{C}^\infty}(U, M)$, i.e., by taking the *functor of points* of M parametrized by smooth open sets. The central result of category theory, called Yoneda's lemma, essentially tells us that the manifold M is completely determined by the functor $\underline{M}$. It is a *sheaf*, meaning that one may paste uniquely parametrized points of M, i.e., a family of morphisms $f_i : U_i \to M$, along a covering $U = \cup_i U_i$ of an open set U, whenever the morphisms are equal on common intersections. Similarly, the group G defines a sheaf

$$\underline{G} : \mathrm{Open}_{\mathcal{C}^\infty}^{op} \to \textsc{Grp}$$

with values in the category of groups.

Now we may define the space $\mathrm{BunCon}_G(M)$ by using parametrized families of principal G-bundles with principal G-connections. More precisely, we will describe it as the sheaf of sets

$$\mathrm{BunCon}_G(M) : \mathrm{Open}_{\mathcal{C}^\infty}^{op} \to \textsc{Sets}$$

that sends an open $U \subset \mathbb{R}^n$ to the set $\mathrm{BunCon}_G(M)(U)$ of pairs (P, A) where P is a principal G-bundle on $M \times U$ (a family of principal bundles on M parametrized by U) and A is a principal G-connection in P relative to U (i.e., a smooth family of principal connections on the fibers of P at points of U, which are principal G-bundles on M).

Now comes an important point: we would like to see $\mathrm{BunCon}_G(M)$ as a space of fields, i.e., of functions on M with values in some space. However, this is not possible in the setting of set-valued sheaves, because the natural parameter space for principal G-bundles is the *classifying stack* BG associated to the group sheaf $\underline{G}$, that is defined as the "homotopical sheaf" with values in groupoids (categories whose only morphisms are isomorphisms)

$$BG : \mathrm{Open}_{\mathcal{C}^\infty}^{op} \to \textsc{Grpd},$$

that sends U to the groupoid $BG(U)$ with one object and morphisms given by $\underline{G}(U) = \mathrm{Hom}_{\mathcal{C}^\infty}(U, G)$. A difficulty in this approach is to define the sheaf condition, because the category GRPD of groupoids should be considered as a 2-category, with 2-morphisms given by natural transformations between functors. Remark that there is a natural functor

$$N : \textsc{Grpd} \to \textsc{SSets}$$

from groupoids to simplicial sets sending a groupoid to its *simplicial nerve*. Concretely, if $BG(U)$ is the groupoid with one object and morphisms given by $\underline{G}(U) = \mathrm{Hom}_{\mathcal{C}^\infty}(U, G)$, then the associated nerve $NBG(U)$ is the simplicial set obtained by setting $NBG(U)_n := \underline{G}(U)^{n-1}$, and the simplicial maps are given by multiplication in $\underline{G}(U)$ and insertions of units. By composing the functor BG with the nerve functor we get a functor

$$NBG : \mathrm{Open}_{\mathcal{C}^\infty}^{op} \to \textsc{SSets}.$$

The "homotopical sheaf" associated to this functor is called the classifying ∞-stack (still denoted BG) of G. A similar but more complicated stack BG_{conn} also exists that classifies parametrized families of pairs (P, A) as above.

We may then define a new stack still denoted $\mathrm{BunCon}_G(M)$ as the mapping stack

$$\mathrm{BunCon}_G(M) := \underline{\mathrm{Hom}}(M, BG_{conn}).$$

Its points parametrized by an open subset $U \subset \mathbb{R}^n$ are essentially given by the (simplicial nerve of the) groupoid of isomorphisms of principal G-bundles with principal connections.

The original formula for our action functional applied to parametrized families of bundles with principal G-connections gives a functional

$$S : \mathrm{BunCon}_G(M) \to \underline{\mathbb{R}},$$

where $\underline{\mathbb{R}}(U) = \mathrm{Hom}(U, \mathbb{R})$.

The usual critical space $\mathrm{Crit}(S) = \{(P, A),\ dS_{(P,A)} = 0\}$ for this action functional is the space of solutions of the Yang-Mills equations. If $X = \mathrm{BunCon}_G(M)$ would be a usual smooth manifold, one may think of the critical space as the intersection

$$\mathrm{Crit}(S) = \mathrm{Im}(dS) \cap T^*_X X \subset T^*X$$

of the image of the differential of S with the zero section of the cotangent bundle of X. In general, this intersection is ill-behaved, and looks like being non-transversal, so that one has to replace the critical space $\mathrm{Crit}(S)$ by the derived intersection

$$\mathbb{R}\mathrm{Crit}(S) = \mathrm{Im}(dS) \overset{h}{\underset{T^*X}{\times}} T^*_X X.$$

One cannot define such a derived smooth space using only open subsets of $\mathbb{R}^n$ as parameters: one has to define a new category of parameters, that contains open subsets but also homotopical infinitesimal extensions of them.

The extension of the category $\mathrm{Open}_{\mathcal{C}^\infty}$ to a bigger category of derived smooth opens is given by a procedure very similar to the one used to define diffeological spaces and smooth ∞-stacks: every open set U defines a *functor of functions*

$$\mathcal{C}^\infty(U) : \mathrm{Open}_{\mathcal{C}^\infty} \to \textsc{Sets}$$

defined by $\mathcal{C}^\infty(U)(V) := \mathrm{Hom}_{\mathcal{C}^\infty}(U, V)$. This functor commutes with products, and sends pullbacks along open inclusions $V \subset W$ to pullbacks. One may think of these two conditions as covariant analogs of the sheaf condition. We will thus define a general smooth algebra A as a functor

$$A : \mathrm{Open}_{\mathcal{C}^\infty} \to \textsc{Sets}$$

that commutes with products and the sends pullbacks along open inclusions $V \subset W$ to pullbacks. With this formulation, it is very easy to give a homotopical generalization of the notion of open subset $U \subset \mathbb{R}^n$: it is given by the notion of a *homotopy smooth algebra* A, that is a functor

$$A : \mathrm{Open}_{\mathcal{C}^\infty} \to \textsc{SSets}$$

that commute homotopically to products and pullbacks along open immersions. We denote $\mathrm{ALG}^h_{\mathcal{C}^\infty}$ the (higher) category of such homotopy smooth algebras. It is possible, if G is a classical real group, to extend the classifying space of G to a (homotopy) functor

$$BG : \mathrm{ALG}^h_{\mathcal{C}^\infty} \to \mathrm{SSETS}$$

on this category of homotopy smooth algebras with values in simplicial sets. Indeed, the sum and product operations $+ : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ and $\times : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ are smooth functions, so that one may use them to define a sum and product on $A(\mathbb{R})$, that makes it a real (homotopy) algebra, and one then defines $G(A)$ as $G(A(\mathbb{R}), +, \times)$. We may then, with some more work, define the derived moduli space of principal bundles with connections BG_{conn}, and get a derived moduli space

$$\mathbb{R}\mathrm{BunConn}_G(M) := \mathbb{R}\underline{\mathrm{Hom}}(M, BG_{conn}) : \mathrm{ALG}^h_{\mathcal{C}^\infty} \to \mathrm{SSETS}.$$

It still carries the Yang-Mills action functional

$$S : \mathbb{R}\underline{\mathrm{Hom}}(M, BG_{conn}) \to \underline{\mathbb{R}},$$

where $\underline{\mathbb{R}} : \mathrm{ALG}_{\mathcal{C}^\infty} \to \mathrm{SSETS}$ is the derived smooth space defined by $\underline{\mathbb{R}}(A) := A(\mathbb{R})$.

If $X = \mathbb{R}\mathrm{BunCon}_G(M)$ is the derived moduli space of principal G-bundles with connections on M, we may now define the derived critical space of the action functional S as the derived intersection

$$\mathbb{R}\mathrm{Crit}(S) = \mathrm{Im}(dS) \underset{T^*X}{\overset{h}{\times}} T^*_X X.$$

As explained above, this derived stack is given by a functor

$$\mathbb{R}\mathrm{Crit}(S) : \mathrm{ALG}^h_{\mathcal{C}^\infty} \to \mathrm{SSETS}$$

that fulfills a sheaf condition. The main output of this construction is that this new space is equipped with a natural (shifted) symplectic form ω, that one may try to quantize using deformation quantization or functional integral methods. This symplectic form may be thought of as an analog of the Peierls bracket, in the case of a theory with gauge invariance.

2 Functorial Geometry and Analysis

We will now give more precise mathematical definitions for the objects considered in the previous chapter.

2.1 Yoneda and the Completion of Categories

Let LEGOS denote a category of simple building blocks for a given geometry (e.g., the category $\mathrm{Open}_{\mathcal{C}^\infty}$ of smooth open subsets $U \subset \mathbb{R}^n$). In general, the category LEGOS have important drawbacks:

1. It does not have enough limits (e.g., solutions of equations, fiber products).
2. It does not have enough colimits (e.g., quotients by group actions).
3. It does not contain "spaces of fields", i.e., functional spaces $\underline{\mathrm{Hom}}(U, V)$.

The solution to these problems was found and used by Grothendieck, Lawvere and Ehresmann in the sities: one may use the Yoneda embeddings

$$\mathrm{LEGOS} \hookrightarrow \underline{\mathrm{Hom}}(\mathrm{LEGOS}^{op}, \mathrm{SETS}) \text{ and } \mathrm{LEGOS}^{op} \hookrightarrow \underline{\mathrm{Hom}}(\mathrm{LEGOS}, \mathrm{SETS})$$

that send a building block U to the set-valued functor of points $\underline{U} = \underline{\mathrm{Hom}}(-, U)$ or the functor of functions $\mathcal{O}(U) := \underline{\mathrm{Hom}}(U, -)$. Yoneda's lemma tells us that the above functors are indeed embeddings, and the main interest of the target categories is that they have arbitrary limits and colimits.

The main interest of this functorial approach to geometry is that it generalizes to homotopical situations, that are necessary to treat obstructions in a geometric way (stacks and derived stacks).

To get sensible generalizations of our building blocs, we want to be able to paste functors of points, and to take tensor products of functors of functions. This is done by the following method:

1. In the functional approach, one defines a generalized algebra to be a *functor of functions*

   $$A : \mathrm{LEGOS} \to \mathrm{SETS}$$

   that commutes with finite products and sends pullbacks along open embeddings to pullbacks. For example

   $$\underline{\mathcal{C}^\infty}(M) : U \mapsto \mathcal{C}^\infty(M, U)$$

   fulfills these conditions.
2. In the punctual approach, one defines a generalized space to be a *functor of points*

   $$X : \mathrm{LEGOS}^{op} \to \mathrm{SETS}$$

   that commutes with pasting of open subsets. For example,

   $$\underline{M} : U \mapsto \mathcal{C}^\infty(U, M)$$

   fulfills these conditions.

One has by definition the right tensor product (no need for completion) for generalized algebras

$$\underline{\mathcal{C}}^\infty(U \times V) \cong \underline{\mathcal{C}}^\infty(U) \otimes \underline{\mathcal{C}}^\infty(V),$$

and the right covering properties or generalized spaces

$$\underline{U \coprod_{U \cap V} V} \cong \underline{U} \coprod_{\underline{U \cap V}} \underline{V}.$$

This allows us to define a manifold M as a functor of point

$$M : \text{LEGOS}^{op} \to \text{SETS}$$

that is a sheaf (i.e., respects pastings) and is equal to the colimit of its representable open subsets $i : \underline{U} \to M$. Every open subset U defines a manifold $\underline{U}$, and one may use pasting to define general manifolds from these basic building blocks. The main output of the punctual approach is that it allows the definition of interesting spaces of fields $\underline{\text{Hom}}(M, N)$ given by smooth spaces of functions between two given manifolds.

In the functional setting, one may define finitely presented rings as functors of functions A that are the coequalizer of two morphisms $f, g : \underline{\mathcal{C}}^\infty(U) \to \underline{\mathcal{C}}^\infty(V)$ between the functor of function of two smooth open subsets. These correspond to formal solution spaces $\{x \in V, f(x) = g(x)\}$ for the equations given by the corresponding smooth functions $f, g : V \to U$. This allows the definition of smooth algebras with nilpotents, such as $\mathcal{C}^\infty(\mathbb{R})/(x^2 = 0)$, that play an important role in the geometric formalization of infinitesimal smooth calculus (called synthetic differential geometry).

Usually, one uses a combination of the functional and the punctual approach, by taking functors of points on functors of functions, to get both infinitesimal and functional spaces.

2.2 *Functorial Analysis*

The jump in abstraction that we have done to do functorial geometry seems to have taken us far from the usual tools of analysis. We will now explain that using functors of points is actually compatible with more classical analysis, if one takes the care of translating things in this new language.

Recall first that the inversion map

$$\begin{aligned} \text{inv} : \mathbb{R} &\to \mathbb{R} \\ x &\mapsto 1/x \end{aligned}$$

is a partially defined function whose definition domain may be computed. We will work with a very general notion of function, and hide the analytic aspects in definition domains. The main interest of this approach is that it gives a clear separation between analytic aspects and geometry, that allows supergeometric and graded generalizations.

Let $\mathcal{C}$ be an ambient category, e.g., $\mathcal{C} = \text{SETS}$ or $\underline{\text{Hom}}(\text{LEGOS}^{op}, \text{SETS})$. Define a *span* $f : X \to Y$ to be a morphism

$$R_f \to X \times Y.$$

A *partial function* $f : X \to Y$ is a span R_f such that $R_f \to X$ is a monomorphism (with image the domain of definition D_f)

Let us look at this general notion by using as a toy model the notion of distribution. We will work with the parametrized space of functions $X = \underline{\text{Hom}}(\mathbb{R}, \mathbb{R})$, defined by

$$X(U) = \text{Hom}_{\mathcal{C}^\infty}(\mathbb{R} \times U, \mathbb{R}),$$

and denote $\mathbb{R}(U) := \text{Hom}_{\mathcal{C}^\infty}(U, \mathbb{R})$.

If $f \in L^1(\mathbb{R})$ is an integrable function, we have a partial function (i.e. natural transformation)

$$\begin{array}{rcl} [f] : X & \to & \mathbb{R} \\ \varphi_u & \mapsto & \int_{\mathbb{R}} f(x)\varphi_u(x)dx, \end{array}$$

whose definition domain is given by Lebesgue domination condition

$$D_f(U) = \{\varphi_u,\ \forall \alpha \text{ loc on } U,\ \exists g_\alpha \in L^1,\ |f(x)\partial_\alpha \varphi_u(x)| \leq g_\alpha(x)\}.$$

The work of the analyst is to find a common definition domain for an interesting big class of functionals. One may now actually define a *distribution* as a (partial) linear function $f : X \to \mathbb{R}$ whose definition domain contains

$$D_{distrib}(U) = \left\{ \varphi_u \;\middle|\; \begin{array}{c} \text{loc. on } U,\ \exists K \subset \mathbb{R} \text{ compact such that} \\ \text{for all } u,\ \text{supp}(\varphi(-,u)) \subset K \end{array} \right\}.$$

2.3 The Critical Space

Now let us consider a variational problem, that is given by the datum of a space M of parameters, a space C of configurations, and a projection $\pi : C \to M$, together with a subspace $H \subset \Gamma(M, C)$ of the space of possible trajectories, called the space of histories, and an action functional $S : H \to \mathbb{R}$.

The main object of interest in classical mechanics is the critical space:

$$\mathrm{Crit}(S) = \{\varphi \in H |\ d_\varphi S = 0\},$$

where S is the action functional (partially) defined by the formula

$$\begin{array}{rl} S : H(U) \to & \mathbb{R}(U) := \mathcal{C}^\infty(U) \\ \varphi_u & \mapsto \int_M L(x, \partial_\alpha \varphi_u(x)) dx \end{array}$$

and with definition domain given by Lebesgue's domination condition

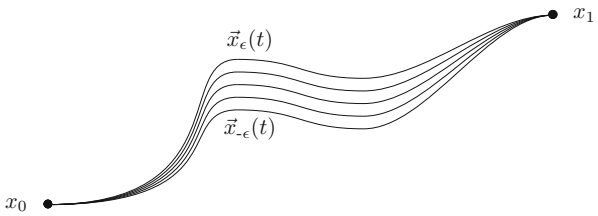
$$D(U) = \{\varphi_u, \exists \text{ locally in } u, g_\beta(x) \in L^1(M), |\partial^u_\beta L(x, \partial_\alpha \varphi_u(x))| \leq g_\beta(x)\}.$$

Remark that if $H = \Gamma(M, C)$, one gets by integration by parts natural boundary conditions $H' \subset H$ such that $\mathrm{Crit}_{|H'}$ is the Euler-Lagrange partial differential equation.

Let us look at the simple example of Newtonian mechanics. Let $M = [0, 1]$ and $C = M \times \mathbb{R}^3$, fix $x_0, x_1 \in C$ and $\vec{v}_0, \vec{v}_1 \in \mathbb{R}^3$ the starting and ending directions. This defines a space of histories H. The action functional of a free particle is

$$S(x) := \int_M \frac{1}{2} m \|\partial_t x(t)\|^2 dt.$$

The computation of the physical trajectories is obtained by making the variation of S along the path



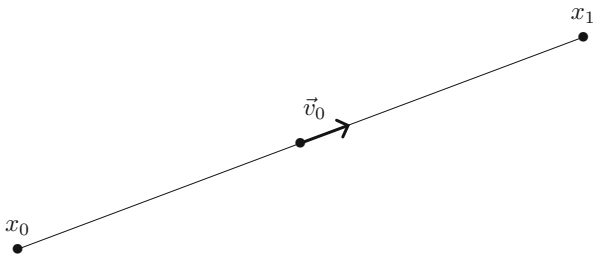
$$\frac{\delta S}{\delta \vec{x}}(x) := \partial_\lambda S(\vec{x}_\lambda)\big|_{\lambda=0}.$$

By integration by parts, one obtains

$$\frac{\delta S}{\delta \vec{x}}(x) = \int_M \langle -m\partial_t^2 x, \partial_\lambda \vec{x} \rangle dt + \cancel{\left[m\langle \partial_t x, \partial_\lambda \vec{x} \rangle \right]_0^1},$$

and this expression is zero for all variations $\vec{x}$ of x if and only if Newton's law $\boxed{m\partial_t^2 x = 0}$ is fulfilled.

We solve the equation given by the fixed initial $(x_0, \vec{v}_0)$ or final $(x_1, \vec{v}_1)$ data.



2.4 Homotopical Geometry

As explained on the example of the pure Yang-Mills formalism, it is necessary for applications to consider also homotopy functors of points and homotopy functors of functions. We will not explain here the full theory but just how one may think of it in analogy with what we have said before.

The main tool in these homotopical generalization is given by the homotopy category of simplicial sets SSETS. A *simplicial set* is a contravariant functor

$$X : \Delta^{op} \to \text{SETS}$$

on the category Δ whose objects are finite ordered non-empty sets $[n] = \{0, \ldots, n\}$ and whose morphisms are increasing maps. Such an objects is completely determined by the family of sets $X([n])$ and by the additional datum of degeneracy and face maps. The category SSETS is actually a homotopy category (also called ∞-category), in which there is a nice notion of homotopy (derived) fiber product and of derived morphism space $\mathbb{R}\underline{\text{Hom}}(X, Y) \in \text{SSETS}$.

One may extend the Yoneda embeddings of our category LEGOS of building blocks for a geometry to Yoneda embeddings

$$\text{LEGOS} \to \underline{\text{Hom}}(\text{LEGOS}^{op}, \text{SSETS}) \text{ and } \text{LEGOS}^{op} \to \underline{\text{Hom}}(\text{LEGOS}^{op}, \text{SSETS}),$$

where $\underline{\text{Hom}}$ denotes the homotopy category of homotopy functors. We then define homotopy algebras (aka derived algebras) as functors

$$A : \text{LEGOS} \to \text{SSETS}$$

that commute homotopically to finite products and open fiber products, and homotopy spaces (aka stacks) as functors

$$X : \text{LEGOS}^{op} \to \text{SSETS}$$

that commute homotopically to nerves of coverings. One may also define derived homotopy spaces as functors

$$X : \text{ALG}^h_{\text{LEGOS}} \to \text{SSETS}$$

on homotopy algebras that commute homotopically to nerves of (hyper-)coverings.

3 $\mathcal{D}$-Geometry and Variational Calculus

An important difficulty that appears in the above formulation of variational calculus is that the spaces we are working with are infinite dimensional, so that there is not good duality between differential forms and tangent vectors. The physicists way of solving this problem is to work only with local quantities, which means, spaces defined by systems of non-linear partial differential equations. We will now explain how these methods can also be formulated in a functorial way.

3.1 $\mathcal{D}$-Spaces and Non-linear PDEs

If M is a smooth manifold, we denote $\mathcal{O} = \mathcal{O}_M$ its sheaf of smooth functions, $\mathcal{D} = \mathcal{D}_M$ the sheaf of local endomorphisms

$$D : \mathcal{O}_M \to \mathcal{O}_M$$

of $\mathcal{O}_M$ generated by $\mathcal{O}_M$ and by the $\mathcal{O}_M$-module Θ_M of derivations.

We will describe linear partial differential systems on M as $\mathcal{D}$-modules and (algebraic) non-linear partial differential systems on M as $\mathcal{D}$-algebras. This gives a coordinate-free treatment of both notions.

A $\mathcal{D}$-algebra is a $\mathcal{D}$-module $\mathcal{A}$ together with an $\mathcal{O}$-algebra structure such that multiplication fulfills Leibniz's rule with respect to derivations $\partial \in \Theta_M$, i.e., we have

$$\partial(fg) = \partial f g + f \partial g.$$

We denote $\text{ALG}_{\mathcal{D}}$ the category of $\mathcal{D}$-algebras on M. If $F(x, u_\alpha) = 0$ is an algebraic partial differential equation on a locally trivial (non-linear) bundle $C \to M$, its

solution space may be computed in every $\mathcal{D}$-algebra $\mathcal{A}$ containing the dependent variable u. This defines a functor

$$\mathrm{Sol}_{F=0}(\mathcal{A}) := \{u \in \mathcal{A},\ F(x, u_\alpha) = 0\}.$$

This functor is a sheaf on $\mathrm{ALG}_{\mathcal{D}}$ with respect to its natural topology, and we will define a general $\mathcal{D}$-space to be such a sheaf

$$F : (\mathrm{ALG}_{\mathcal{D}})^{op} \to \mathrm{SETS}.$$

There is a very rich geometry for such spaces, that is more complicated than the smooth geometry we have explained before, because of the fact that $\mathcal{D}$ is a non-commutative ring.

The solution space $\mathrm{Sol}_{F=0}$ is representable by the $\mathcal{D}$-algebra $\mathrm{Jet}(\mathcal{O}_C)/(F)$, i.e., there is a natural isomorphism

$$\mathrm{Sol}_{F=0}(-) \cong \mathrm{Hom}_{\mathrm{ALG}_{\mathcal{D}}}(\mathrm{Jet}(\mathcal{O}_C)/(F), -).$$

3.2 Variational Calculus

If $\mathcal{A}$ is a $\mathcal{D}$-algebra, we now denote

$$\mathrm{DR}(\mathcal{A}) := \Omega^n_M \overset{\mathbb{L}}{\otimes}_{\mathcal{D}} \mathcal{A}.$$

This is the de Rham cohomology of the given $\mathcal{D}$-algebra.

There is a natural integration pairing between $H_{*,c}(M)$ and $h^*(\mathrm{DR}(\mathcal{A}))$ with values in differential forms on the smooth space $\Gamma(M, C)$ of sections of the given bundle. We define local functionals as elements in

$$h(\mathcal{A}) := h^0(\mathrm{DR}(\mathcal{A})).$$

These cohomology classes represent true functionals of the form

$$S(\varphi) = \int_M L(x, \varphi(x), \partial_\alpha \varphi(x))dx.$$

The advantage of the cohomological formulation is that it allows to do all computations purely in differential terms, à la Lagrange. In particular, we can define the Euler-Lagrange equation purely algebraically by the following recipe.

Let $\mathcal{A} := \mathrm{Jet}(\mathcal{O}_C)$ be the algebra of coordinates on the jet space of the given bundle $C \to M$. Let $d : \mathcal{A} \to \Omega^1_{\mathcal{A}}$ be the universal $\mathcal{D}$-derivation on $\mathcal{A}$, and denote

$$\Theta_{\mathcal{A}} := \mathrm{Hom}_{\mathcal{A}[\mathcal{D}]}(\Omega^1_{\mathcal{A}}, \mathcal{A}[\mathcal{D}]).$$

Remark that we have used $\mathcal{D}$-duality, and not only $\mathcal{A}$-duality. This is what makes $\mathcal{D}$-geometry and its differential calculus a bit more intricate than usual differential calculus on smooth manifolds. Still, there is an interior product map

$$i_{dS} : \Theta^{\ell}_{\mathcal{A}} \to \mathcal{A}$$

with $\Theta^{\ell}_{\mathcal{A}} := \Omega^n \otimes_{\mathcal{O}} \Theta_{\mathcal{A}}$ is the left $\mathcal{D}$-module associated to the right $\mathcal{D}$-module of local vector field densities $\Theta_{\mathcal{A}}$. If we denote $\mathcal{I}_S := \mathrm{im}(i_{dS})$ the critical $\mathcal{D}$-ideal in $\mathcal{A}$, given by the image of the interior product map, the critical space is given by the Euler-Lagrange $\mathcal{D}$-space

$$\mathrm{Crit}_{\mathcal{D}}(S) = \mathrm{Spec}(\mathcal{A}/\mathcal{I}_S).$$

This is a $\mathcal{D}$-space over M whose solution space (if one chooses nice boundary conditions for the action functional) is given by the smooth critical space $\mathrm{Crit}(S)$ that we have already described before.

Remark that we have also a differential graded (derived) $\mathcal{D}$-space called the derived critical space

$$\mathbb{R}\mathrm{Crit}(S) = \mathbb{R}\mathrm{Spec}_{\mathcal{D}}(\mathrm{Sym}_{\mathcal{A}-dg}(\Theta^{\ell}_{\mathcal{A}} \xrightarrow{i_{dS}} \mathcal{A})).$$

It is a homotopy sheaf (stack) on the category of differential graded $\mathcal{D}$-algebras on M with values in the ∞-category SSETS of simplicial sets. The nice property of this derived space is that it always has a Poisson structure, given by the action of derivations on $\mathcal{A}$ and the Lie bracket on derivations (Schouten-Nijenhuis bracket).

4 Homotopical Poisson Reduction of Gauge Theories

Now we arrive to the functorial $\mathcal{D}$-geometric formulation of the standard method used by physicists to prepare a gauge system for being quantized, called the Batalin-Vilkovisky formalism.

An intrinsic definition of gauge symmetries may be given by setting

$$\mathfrak{h}_S := \Theta_{\mathrm{Crit}(S)/\mathbb{R}\mathrm{Crit}(S)},$$

where $\mathrm{Crit}(S) \to \mathbb{R}\mathrm{Crit}(S)$ is the natural inclusion, that we may think of as a the inclusion of the critical space into its homotopy tubular neighborhood. This gives a

natural homotopy Lie algebra structure on $\mathfrak{h}_S$. Suppose we may choose a retraction $r : \mathbb{R}\mathrm{Crit}(S) \to \mathrm{Crit}(S)$ such that

$$\mathfrak{g}_S := \Theta_{\mathbb{R}\mathrm{Crit}(S)/\mathrm{Crit}(S)} \to \Theta_{\mathbb{R}\mathrm{Crit}(S)}$$

induces an Hamiltonian flow on the Poisson (actually odd symplectic) $\mathcal{D}$-space $\mathbb{R}\mathrm{Crit}(S)$. This will be called a Hamiltonian retraction. Then we may define the homotopical Poisson reduction as the Poisson reduction of the derived critical space by this Hamiltonian action. This essentially corresponds to the following more explicit construction.

Define a graded module $\mathfrak{g}_S$ of gauge symmetries for $S \in h(\mathcal{A})$ as a generating module of a cofibrant resolution

$$\mathcal{A}' = (\mathrm{Sym}(\mathfrak{g}_S[2] \oplus \Theta^{\ell}_{\mathcal{A}}[1] \oplus \mathcal{A}), d) \xrightarrow{\sim} \mathcal{A}/\mathcal{I}_S$$

whose components are free $\mathcal{A}[\mathcal{D}]$-modules of finite rank.

If $\mathfrak{g}$ is in degree zero, the local Lie bracket of local vector fields induces

$$[-,-] : \mathfrak{g}_S \boxtimes \mathfrak{g}_S \to \Delta_* \Theta_{\mathcal{A}}.$$

Batalin and Vilkovisky define a "homotopical Poisson reduction"

$$\mathrm{Crit}(S)\underset{\mathbb{L}}{/}\mathfrak{g} := \mathbb{R}\mathrm{Spec}(\mathcal{A}/\mathcal{I}_S)\underset{\mathbb{L}}{/}\mathfrak{g},$$

by solving $\{S_{cm}, S_{cm}\} = 0$ in the local bigraded Poisson algebra

$$\mathcal{A}_{BV} = \mathrm{Sym}_{bigrad}\left(\begin{bmatrix} \mathfrak{g}_S[2] \oplus \Theta^{\ell}_{\mathcal{A}}[1] \oplus & \mathcal{A} \\ & \oplus \\ & {}^t\mathfrak{g}_S^{\circ}[-1] \end{bmatrix}\right).$$

To quantize, on needs to fix a (derived) Lagrangian in the odd Poisson BV space

$$X_{BV} = \mathbb{R}\mathrm{Spec}(\mathcal{A}_{BV}, \{S_{cm}, -\}).$$

In practice, one may add generators with trivial cohomology so that the derived Lagrangians become graded.

Our main input is to give a precise mathematical formulation of the BV formalism, that allows to understand precisely the finiteness conditions the are necessary to its validity.

Theorem 1 *A supersymmetric gauge theory $S \in h(\mathcal{A})$ (with the right finiteness conditions) allows to define $S_{cm} \in h(\mathcal{A}_{BV})$ fulfilling the classical master equation*

$$\{S_{cm}, S_{cm}\} = 0.$$

In our book, we also give a detailed and geometric construction, using functors of points, of the gauge fixing procedure, in full generality. Our main motivation is to better understand perturbative quantization à la Epstein-Gläser in chiral algebras using microlocal analysis.

5 Quantizing Gauge Theories

The output of the homotopical Poisson reduction of gauge theories, also called the Batalin-Vilkoviski formalism, is a derived Poisson $\mathcal{D}$-space X_{BV} over the parameter manifold M, whose functions correspond, in the physicists' language, to local functionals in the fields and antifields variables. There are now various ways to formalize mathematically what it means to quantize this Poisson $\mathcal{D}$-space.

5.1 The Deformation Quantization Approach

The most natural approach to quantize the Batalin-Vilkovisky space, from the point of view of derived $\mathcal{D}$-geometry, is given by the setting of Chiral algebras and factorization spaces, that is a geometric formulation of the physical notion of operator product expansion: using multijets instead of jets, one may extend the derived $\mathcal{D}$-space X_{BV} to a $\mathcal{D}$-space X_{BV}^{Ran} on the Ran (configuration) space, that is defined by

$$\mathrm{Ran}(M) := \mathrm{colim}_{I \twoheadrightarrow J} M^I$$

where the colimit is taken along diagonals $\Delta(\pi) : M^J \to M^I$ associated to surjections $\pi : I \twoheadrightarrow J$ of finite sets. One may think of X_{BV}^{Ran} as a space that encodes power series expansions along field derivatives at multiple points, in a way similar to the way the jet space encodes power series expansions along field derivatives at points.

The operation

$$\mathrm{union} : \mathrm{Ran}(M) \times \mathrm{Ran}(M) \to \mathrm{Ran}(M)$$

of union of subsets and

$$j : (\mathrm{Ran}(M) \times \mathrm{Ran}(M))_{disj} \to \mathrm{Ran}(M) \times \mathrm{Ran}(M)$$

of inclusion of disjoint pairs induce a chiral monoidal structure on $\mathcal{D}$-modules on $\mathrm{Ran}(M)$ given by

$$\otimes^{ch} := \mathrm{union}_* j_* j^* (- \boxtimes -).$$

One may show that the algebra of functions on X_{BV}^{Ran} defines a Lie algebra in the category of $\mathcal{D}$-modules on $\mathrm{Ran}(M)$ for the chiral monoidal structure, that is commutative, in some sense. The quantization problem is then to deform this Lie algebra structure to a non-commutative one with associated semi-classical bracket the given Poisson bracket on X_{BV}.

Let us illustrate this in the simple case of a particle depending only on a time variable in $M = \mathbb{R}$. A chiral Lie algebra on $\mathbb{R}$ is simply an associative algebra, and it is commutative if and only if the associative algebra is commutative. So in this one parameter case, the aim of quantization is to deform a commutative algebra to an associative one.

One may also understand the deformation quantization of Poisson manifolds in this setting by using chiral algebras on the (compactified) Poincaré Half place

$$\bar{\mathbb{H}} := \{z \in \mathbb{Z},\ \mathrm{Im}(z) \geq 0\}.$$

Indeed, every Poisson manifold $(X, \{-,-\})$ defines a field theory on $\bar{\mathbb{H}}$ called the Poisson sigma model. By quantizing it by deformation, one gets a chiral algebra on $\bar{\mathbb{H}}$ that may be pulled back to the real line $\mathbb{R}$, to get an associative algebra that will be the deformation quantization of the given Poisson manifold.

If we want to get to a more physical setting, we may start with a global hyperbolic spacetimes $M = \mathbb{R} \times M_0$. The quantization of the Batalin-Vilkovisky space of a classical gauge theory on M would give a chiral algebra on M (i.e., a Lie algebra for the chiral structure in $\mathcal{D}$-modules on $\mathrm{Ran}(M)$ supported on M) whose pullback on $\mathbb{R} \times \{x_0\}$ will be a chiral algebra on $\mathbb{R}$, that is known to be an associative algebra. Now if we fix time t_0 and pullback the given chiral algebra on $\{t_0\} \times M_0$, we get a chiral algebra on M_0, that is known to be, if $M_0 \cong \mathbb{R}^3$, an E_3-algebra (aka 3-associative homotopy algebra). This additional information (an actually the full 4-dimensional chiral algebra structure) should be thought of as an algebraic analog of the physicists' operator product expansion.

5.2 Relation with Perturbative Quantum Field Theory

Another approach to the quantization of the Batalin-Vilkovisky $\mathcal{D}$-space of fields is given by the causal approach of Epstein-Glaser-Brunetti-Fredenhagen. One needs for this to develop a gauge fixing procedure, which starts by giving the additional datum of a Batalin-Vilkovisky graded bundle E_{BV} over M whose sections correspond the additional fields. We now work with graded spaces, whose building blocks are algebras of the form $\Gamma(U, \mathrm{Sym}^*(V))$ for V a graded bundle on an open subset U of $\mathbb{R}^n$.

The Batalin-Vilkovisky function S_{cm} then gives a degree 0 functional

$$S_{cm} : \Gamma(M, E_{BV}) \to \underline{\mathbb{R}}.$$

One then needs to fix the gauge, by using a Lagrangian $\mathcal{D}$-subspace X_{fields} of the space X_{BV}, represented by another bundle E_{fields} on M and a morphism

$$L = \Gamma(M, E_{fields}) \to \Gamma(M, E_{BV}).$$

The composition of this map with the Batalin-Vilkovisky functional gives the so-called gauge-fixed action

$$S_{gf} : L = \Gamma(M, E_{fields}) \to \underline{\mathbb{R}},$$

and one should suppose that it is non-degenerate. In the free field case, this means that one may invert the corresponding linear differential operator, or at least, find a parametrix for it.

This action functional is now the one that should be used for the perturbative approach to quantum field theory, using functional integrals. For this, one needs to decompose the local gauge fixed action functional as a sum of a free part and an interaction part with a small parameter, and write formal Gaussian integrals associated to it. This leads to the renormalization problem. The renormalization theory may then be formalized mathematically using the Epstein-Glaser formalism, developed further by Brunetti-Fredenhagen and Rejzner (in the case of gauge theories).

Reference

1. F. Paugam, *Towards the Mathematics of Quantum Field Theory* (Springer, Cham, 2014)

A Solvable Four-Dimensional QFT

Harald Grosse and Raimar Wulkenhaar

Contents

Abstract We review a sequence of papers in which we show that the quartic matrix model with an external matrix is exactly solvable in terms of the solution of a non-linear integral equation. The interacting scalar model on four-dimensional Moyal space is of this type, and our solution leads to the construction of Schwinger functions. Taking a special limit leads to a QFT on $\mathbb{R}^4$ which satisfies growth property, covariance and symmetry. There is numerical evidence for reflection positivity of the 2-point function for a certain range of the coupling constant.

H. Grosse (✉)
Fakultät für Physik, Universität Wien, Boltzmanngasse 5, A-1090 Wien, Austria
e-mail: harald.grosse@univie.ac.at

R. Wulkenhaar
Mathematisches Institut der Westfälischen Wilhelms-Universität, Einsteinstraße 62, D-48149 Münster, Germany
e-mail: raimar@math.uni-muenster.de

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_8

Keywords Quantum field theory • Solvable models • Schwinger-Dyson techniques • Fixed point methods

Mathematics Subject Classification (2010). 81T16, 81T08, 39A99, 45E05

1 Prehistory

In December 1999, Minwalla, van Raamsdonk and Seiberg demonstrated [31] that quantum field theories on noncommutative spaces, although nice at one-loop order [26, 30], generate a severe problem in higher loops (UV/IR-mixing). The mechanism was thoroughly analysed in two papers by Chepelev and Roiban [6, 7].

In summer 2002 we started a final attempt to make sense of noncommutative quantum field theories. Quantum field theory involves delicate limiting procedures and it was not completely clear that the manipulations of oscillating integrals are mathematically justified. A prerequisite to rigorous quantum field theory is to put the model into finite volume and to restrict it to finite energy. Inspired by a discussion with Thomas Krajewski, we tried to analyse the Moyal models in analogy to Polchinski's renormalisation proof [35] of the $\lambda\phi_4^4$-model using exact renormalisation group equations. This approach has clear infrared and ultraviolet cut-offs and proves rigorous bounds for the amplitude of Feynman graphs. All this fails for oscillating integrals. The programme was rescued thanks to a hint by José Gracia-Bondía who introduced us to his work [12, 42] on the matrix basis of the Moyal space. We briefly collect the most relevant results.

The Moyal plane is the space of Schwartz class functions equipped with the noncommutative but associative product

$$(f\star g)(x)=\int_{\mathbb{R}^d\times\mathbb{R}^d}\frac{dy\,dk}{(2\pi)^d}f\big(x+\tfrac{1}{2}\Theta k\big)\,g\big(x+y\big)\,e^{\mathrm{i}\langle k,y\rangle}\ ,\quad f,g\in\mathcal{S}(\mathbb{R}^d)\ . \tag{1}$$

Here, $\Theta=-\Theta^t\in M_d(\mathbb{R})$ is a skew-adjoint constant matrix. We assume $d=2$ for simplicity. The Gaußian

$$f_{00}(x)=2\mathrm{e}^{-\frac{1}{\theta}(x_1^2+x_2^2)} \tag{2}$$

is an *idempotent* for the $\star$-product, $(f_{00}\star f_{00})(x)=f_{00}(x)$. We consider creation and annihilation operators

$$a=\frac{1}{\sqrt{2}}(x_1+\mathrm{i}x_2)\ ,\qquad \bar a=\frac{1}{\sqrt{2}}(x_1-\mathrm{i}x_2)\ . \tag{3}$$

One shows $a \star f_{00} = 0$ and $f_{00} \star \bar{a} = 0$ and defines

$$f_{mn} := \frac{1}{\sqrt{n!m!}\,\theta^{m+n}}\, \bar{a}^{\star m} \star f_{00} \star a^{\star n} \,. \tag{4}$$

The f_{mn} can be expressed in terms of Laguerre polynomials. The commutation rule $[a, \bar{a}] = \theta$ leads to

$$(f_{mn} \star f_{kl})(x) = \delta_{nk} f_{ml}(x) \,. \tag{5}$$

The multiplication rule (5) identifies the $\star$-product with the ordinary matrix product; in fact there this gives an isomorphism of Fréchet algebras between Schwartz functions with $\star$-product on one hand and the product of matrices with rapidly decaying entries on the other hand [12]. Finally, one checks

$$\int d^2x f_{mn}(x) = 2\pi\theta\delta_{mn} \,. \tag{6}$$

Expanding $\phi(x_1, \ldots, x_4) = \sum_{\underline{m},\underline{n}\in\mathbb{N}^2} \Phi_{\underline{mn}} f_{m_1 n_1}(x_1, x_2) f_{m_2 n_2}(x_3, x_4)$, now in $d = 4$ dimensions, the $\phi_4^{\star 4}$-interaction becomes a matrix product,

$$\int d^4x\, (\phi \star \phi \star \phi \star \phi)(x) = (2\pi\theta)^2 \sum_{\underline{k},\underline{l},\underline{m},\underline{n}\in\mathbb{N}^2} \Phi_{\underline{kl}} \Phi_{\underline{lm}} \Phi_{\underline{mn}} \Phi_{\underline{nk}} \,. \tag{7}$$

The prize is a complicated kinetic term

$$\int d^4x\, (\phi \star (-\Delta)\phi)(x) = (2\pi\theta)^2 \sum_{\underline{k},\underline{l},\underline{m},\underline{n}\in\mathbb{N}^2} \Delta_{\underline{kl};\underline{mn}} \Phi_{\underline{kl}} \Phi_{\underline{mn}} \tag{8}$$

for a certain integral kernel $\Delta_{\underline{kl};\underline{mn}}$ of the Laplace operator. Angular momentum conservation restricts to $\delta_{k_i+m_i, l_i+n_i}$. Then in both pairs $\underline{kn}$ and $\underline{ml}$ the kernel is, in two dimensions, a tri-diagonal band matrix, in general a sum of local interaction $\sim \delta_{\underline{lm}}\delta_{\underline{kn}}$ plus nearest neighbour interaction $\delta_{k_i, m_i \pm 1}$. To obtain Feynman rules we must invert the kernel operator $\Delta_{\underline{kl};\underline{mn}}$ and then introduce a cut-off. This was first done with a computer and small matrix cut-off $\mathcal{N}$. We found that the graphs do not behave well, for a surprising reason. The local part of $\Delta_{\underline{kl};\underline{mn}}$ was fine, but this was destroyed by the nearest-neighbour terms. In December 2002 we came up with the following working hypothesis: *Let us scale the nearest neighbours down by a factor* < 1. Then everything worked (for the computer).

We asked ourselves what operator on x-space corresponds to the weakened nearest neighbours. The answer is: an additional harmonic oscillator potential

$$\int d^4x\, (\phi \star (-\Delta)\phi)(x) \mapsto \int d^4x\, (\phi \star (-\Delta + \Omega^2 \|2\Theta^{-1}x\|^2 \phi))(x) \,, \tag{9}$$

where $\Omega^2 < 1$. By January 2004 we achieved:

Theorem 1.1 ([16]+[15]) *The action*

$$S = \int_{\mathbb{R}^4} dx \Big(\frac{Z}{2} \phi (-\Delta + \Omega^2 \|2\Theta^{-1} x\|^2 + \mu^2) \phi + \frac{Z^2 \lambda}{4} \phi \star \phi \star \phi \star \phi \Big)(x) \qquad (10)$$

is renormalisable to all orders in perturbation theory by suitable dependence of Z, μ, λ, Ω *on cut-off and normalisation.*

A few remarks:

- Translation invariance is explicitly broken. This will be repaired in the next sections. On the other hand, the action is covariant under a duality found by Langmann and Szabo [28]. This duality consists in exchanging the function and its Fourier transform $\phi(x) \leftrightarrow \hat{\phi}(p)$, position and momentum $2\Theta^{-1} x \leftrightarrow p$ and then in reverting to the old variables by a modified Fourier transform with alternating $\pm$i in the phase. This transform leaves the interaction $\int dx\, (\phi \star \phi \star \phi \star \phi)(x)$ invariant, and it exchanges $\int dx\, (\phi \star (-\Delta \phi))(x)$ with $\int dx\, (\phi \star (\|2\Theta^{-1} x\| \phi))(x)$. The action (10) is Langmann-Szabo covariant: $S[\mu, \lambda, \Omega] \mapsto \Omega^2 S[\frac{\mu}{\Omega}, \frac{\lambda}{\Omega^2}, \frac{1}{\Omega}]$.
- With some effort one can show [15] that all planar graphs with >4 external legs and all non-planar graphs (amplitude $\sim \Omega^{-n}$) are finite. But this is not enough, we need the analogue of locality. For instance, in the effective action we get contributions to the 2-point function $\sum G_{\underline{k}\underline{l};\underline{m}\underline{n}} \Phi_{\underline{k}\underline{l}} \Phi_{\underline{m}\underline{n}}$ with (up to angular momentum conservation) any $\underline{k}, \underline{l}, \underline{m}, \underline{n}$. But for renormalisability only the local terms and the nearest-neighbour terms are allowed to diverge, and a single subtraction at vanishing indices must remove the divergence. This turned out to be true. A key step in the proof was an exact diagonalisation of the $\Delta_{\underline{k}\underline{l};\underline{m}\underline{n}}$-kernel via Meixner polynomials. These are expressed in terms of hypergeometric functions so that we were able to control the non-local terms.

During a visit of ESI early 2004 we computed the one-loop β-function of that model. We got explicit formulae, expressed in terms of hypergeometric functions, showing that both Ω and λ flow, that $\beta_\lambda = \mathcal{N} \frac{d\lambda}{d\mathcal{N}}$ is positive but vanishes at $\Omega = 1$ [14]. At the end of a presentation of these results in Marseille, David Broadhurst pointed out a remarkable coincidence with these formulae: The flow is such that $\frac{\Omega^2}{\lambda}$ remains constant! Since Ω flows into its fixed point $\Omega_\infty = 1$, the running coupling constant stays bounded over all scales, with finite $\lambda_\infty = \frac{\lambda_0}{\Omega_0^2}$. There is no Landau ghost [17]!

Shortly later, one of us (RW) had the chance to explain these results to Vincent Rivasseau who visited the MPI Leipzig. A simple model without Landau ghost was something he searched for long time. So we started a collaboration with the aim to construct this model non-perturbatively [36]. Vincent Rivasseau infected his scientific environment with this idea: Jacques Magnen, Margherita Disertori, Jean-Christophe Wallet and a growing number of young people: Fabien Vignes-Tourneret, Razvan Gurau, Adrian Tanasa, Zhituo Wang, Axel de Goursac and in

some parts also Thomas Krajewski. There was a first joint publication on multiscale analysis [38], but then Rivasseau's group was much faster: they reproved the renormalisation theorem in position space [23], derived the Symanzik polynomials [22], extended the method to the Gross-Neveu model [43] and so on [37].

The most important achievement started with a remarkable three-loop computation of the β-function by Margherita Disertori and Vincent Rivasseau [8] in which they confirmed that at $\Omega = 1$, β vanishes to three-loop order. The great idea was to work in the matrix basis but take advantage of the fact that the Δ-kernel is local for $\Omega = 1$. Eventually, M. Disertori, R. Gurau, J. Magnen and V. Rivasseau proved in [9] that the β-function vanishes to all orders in perturbation theory. The key step consists in an ingenious combination of Ward identities with Schwinger-Dyson equation which they borrowed from a work of Benfatto and Mastropietro [1] on one-dimensional Fermi systems.

We felt that the result of [9] goes much deeper: Using these tools it must be possible to solve the model!

2 Details of the Solution

2.1 Reformulation as Matrix Model

We follow the Euclidean approach, starting from a partition function with source term $\mathcal{Z}[J]$, which itself involves the action functional of the model. For concreteness, let us look at the $\lambda\phi_4^4$-model defined by the action functional

$$S[\phi] = \int_{\mathbb{R}^4} dx \left\{ \frac{1}{2}\phi(x) \cdot (-\Delta + \mu^2)(\phi(x)) + \frac{\lambda}{4}\big(\phi(x)\big)^4 \right\} . \tag{11}$$

It is absolutely crucial that, as in any rigorous construction, this action functional cannot be taken as the naïve action $S[\phi]$. We have to *regularise* the action, namely to place it into finite volume V and introduce an energy cut-off Λ. These must be removed in the very end to restore symmetry. For $V \to \infty$ we study the free energy density $\frac{1}{V}\log(\mathcal{Z}[J])$ and functions derived from that. The limit $\frac{1}{\Lambda} \to 0$ is achieved by the renormalisation philosophy. There is a renormalisation group flow of effective actions down in Λ, and the key step is to impose mixed boundary conditions: finitely many relevant and marginal couplings are fixed at $\Lambda_R = 0$, the infinitely many irrelevant couplings at $\Lambda \to \infty$. This involves an inversion of the renormalisation group flow which typically requires perturbation theory.

Finite volume is actually a compactification of the underlying geometry. A more sophisticated method than putting the model into a box is to add in (11) a harmonic oscillator potential $-\Delta \mapsto H := -\Delta + \omega^2\|x\|^2$. The result is the same, the resolvent $(H + \mathrm{i})^{-1}$ is a compact operator (with discrete spectrum), and the D-dimensional spectral volume is proportional to $\omega^{-\frac{D}{2}}$.

A well-known restriction of the energy density consists in introducing a lattice of spacing $a = \frac{1}{\Lambda}$. This is the heart of the lattice gauge theory approach [46] to quantum chromodynamics. As action one takes, for example, Wilson's plaquette action, which is *non-local* but converges for $a \to 0$ to the local Yang-Mills action. We choose the Moyal product as our preferred non-locality:

$$S_{\Omega,\theta}[\phi] = \frac{1}{64\pi^2}\int d^4x\Big(\frac{Z}{2}\phi\star\big(-\Delta+\Omega^2_{bare}\|2\Theta^{-1}x\|^2+\mu^2_{bare}\big)\phi + \frac{\lambda_{bare}Z^2}{4}\phi\star\phi\star\phi\star\phi\Big)(x)\ . \tag{12}$$

We pass to matrix representation; the energy cut-off is then the restriction to finite matrices:

$$S^{\mathcal{N}}_{\Omega,\theta}[\Phi] = \Big(\frac{\theta}{4}\Big)^2 \sum_{\underline{k},\underline{l},\underline{m},\underline{n}\in\mathbb{N}^2_{\mathcal{N}}} \Big(\frac{Z}{2}\Phi_{\underline{k}\underline{l}}(\Delta^{(\Omega)}_{\underline{k}\underline{l};\underline{m}\underline{n}} + \mu^2_{bare}\delta_{\underline{k}\underline{n}}\delta_{\underline{l}\underline{m}})\Phi_{\underline{m}\underline{n}} + \frac{Z^2\lambda_{bare}}{4}\Phi_{\underline{k}\underline{l}}\Phi_{\underline{l}\underline{m}}\Phi_{\underline{m}\underline{n}}\Phi_{\underline{n}\underline{k}}\Big)\ . \tag{13}$$

This action is used to define the partition function. We should perform the renormalisation and then take the limits $\mathcal{N}\to\infty$, $\theta\to 0$ and $\Omega\to 0$ to rigorously define the $\lambda\phi^4_4$-model. This is not what we do; we take $\Omega = 1$. At first sight, this cuts all ties to translation invariance. The only chance to kill the oscillator potential for $\Omega = 1$ is to let $\theta\to\infty$. This is a highly singular limit in (1), although already mentioned in [31] as 'stringy'. We were able to make sense of this limit first for matrices [18] but later in position space [20], and surprisingly it not only restores translation invariance but also full rotation invariance.

At $\Omega = 1$ the kernel of the Schrödinger operator is local,

$$\Delta^{(\Omega=1)}_{\underline{k}\underline{l};\underline{m}\underline{n}} = \frac{|\underline{m}|+|\underline{n}|+2}{\sqrt{V}}\ ,\quad |\underline{m}| := m_1+m_2 \text{ for } \underline{m}=(m_1,m_2)\ ,\quad V=\Big(\frac{\theta}{4}\Big)^2\ .$$

This allows us to write the action as

$$S[\Phi] = V\,\mathrm{tr}\Big(E\Phi^2+\frac{Z^2\lambda}{4}\Phi^4\Big)\ ,\quad E=(E_{\underline{m}}\delta_{\underline{m}\underline{n}})\ ,\quad E_{\underline{m}} = Z\Big(\frac{|\underline{m}|}{\sqrt{V}}+\frac{\mu^2_{bare}}{2}\Big)\ . \tag{14}$$

We view E as unbounded operator on Hilbert space which is positive, selfadjoint and has compact resolvent. Adding a source term to the action, we define the partition function as

$$\mathcal{Z}[J] = \int \mathcal{D}[\Phi]\ \exp(-S[\Phi]+V\,\mathrm{tr}(\Phi J))\ , \tag{15}$$

where $\mathcal{D}[\Phi]$ is the extension of the Lebesgue measure from finite-rank operators to the Hilbert-Schmidt class and J a test function matrix. In the sequel we use simplified notation $\underline{m} \mapsto m$ and $\mathbb{N}_{\mathcal{N}}^2 \mapsto I$.

2.2 Ward Identity and Topological Expansion

There is a subgroup of unitary operators U on Hilbert space such that the transformed operator $\tilde{\Phi} = U\Phi U^*$ belongs to the same class as Φ. This implies

$$\int \mathcal{D}[\Phi]\ \exp(-S[\Phi] + V\,\mathrm{tr}(\Phi J)) = \int \mathcal{D}[\tilde{\Phi}]\ \exp(-S[\tilde{\Phi}] + V\,\mathrm{tr}(\tilde{\Phi} J))\ .$$

Unitary invariance $\mathcal{D}[\tilde{\Phi}] = \mathcal{D}[\Phi]$ of the Lebesgue measure leads to

$$0 = \int \mathcal{D}[\Phi] \left\{ \exp(-S[\Phi] + V\,\mathrm{tr}(\Phi J)) - \exp(-S[\tilde{\Phi}] + V\,\mathrm{tr}(\tilde{\Phi} J)) \right\}\ .$$

Note that the integrand $\{\dots\}$ itself does not vanish because $\mathrm{tr}(E\Phi^2)$ and $\mathrm{tr}(\Phi J)$ are not unitarily invariant; we only have $\mathrm{tr}(\Phi^4) = \mathrm{tr}(\tilde{\Phi}^4)$ due to $UU^* = U^*U = \mathrm{id}$ together with the trace property. Linearisation of U about the identity operator leads to the *Ward identity*

$$0 = \int \mathcal{D}[\Phi] \left\{ E\Phi\Phi - \Phi\Phi E - J\Phi + \Phi J \right\} \exp(-S[\Phi] + V\,\mathrm{tr}(\Phi J))\ . \tag{16}$$

We can always choose an orthonormal basis where E is diagonal (but J is not). Since E is of compact resolvent, E has eigenvalues $E_a > 0$ of finite multiplicity μ_a. We thus label the matrices by an enumeration of the (necessarily discrete) eigenvalues of E and an enumeration of the basis vectors of the finite-dimensional eigenspaces. Writing Φ in $\{\dots\}$ of (16) as functional derivative $\Phi_{ab} = \frac{\partial}{V \partial J_{ba}}$, we have thus proved (first obtained in [9]):

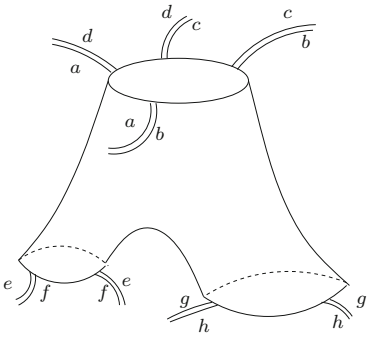
Proposition 2.1 *The partition function $\mathcal{Z}[J]$ of the matrix model defined by the external matrix E satisfies the $|I| \times |I|$ Ward identities*

$$0 = \sum_{n \in I} \left(\frac{(E_a - E_p)}{V} \frac{\partial^2 \mathcal{Z}}{\partial J_{an} \partial J_{np}} + J_{pn} \frac{\partial \mathcal{Z}}{\partial J_{an}} - J_{na} \frac{\partial \mathcal{Z}}{\partial J_{np}} \right)\ . \tag{17}$$

The compactness of the resolvent of E implies that at the expense of adding a measure $\mu_{[m]} = \dim \ker(E - E_m \mathrm{id})$, we can assume that $m \mapsto E_m$ is injective.

In a perturbative expansion, Feynman graphs in matrix models are *ribbon graphs*. Viewed as simplicial complexes, they encode the topology (B, g) of a genus-g Riemann surface with B boundary components. The kth boundary face is

characterised by $N_k \geq 1$ external double lines to which we attach the source matrices J. See e.g. [15]. Since E is diagonal, the matrix index is conserved along each strand of the ribbon graph. Therefore, the right index of J_{ab} coincides with the left index of another J_{bc}, or of the same J_{bb}. Accordingly, the kth boundary component carries a cycle $J_{p_1 \dots p_{N_k}} := \prod_{j=1}^{N_k} J_{p_j p_{j+1}}$ of N_k external sources, with $N_k + 1 \equiv 1$. Here is a drawing for a ($B = 3, g = 0$) Riemann surface with cycles of lengths $N_1 = 4$, $N_2 = 2, N_3 = 2$:



$$(J_{ab}J_{bc}J_{cd}J_{da})\,(J_{ef}J_{fe})\,(J_{gh}J_{hg})$$

We had discussed that only $\frac{1}{V}\log \mathcal{Z}[J]$, not $\mathcal{Z}[J]$ itself, can have an infinite volume limit. Consequently we *define* $\log \mathcal{Z}[J]$ as an expansion according to the cycle structure:

$$\log \frac{\mathcal{Z}[J]}{\mathcal{Z}[0]} = \sum_{B=1}^{\infty} \sum_{1 \leq N_1 \leq \dots \leq N_B}^{\infty} \sum_{p_1^\beta, \dots, p_{N_\beta}^\beta \in I} \frac{V^{2-B}}{S_{N_1 \dots N_B}} G_{|p_1^1 \dots p_{N_1}^1 | \dots | p_1^B \dots p_{N_B}^B|} \times \prod_{\beta=1}^{B} \Big(\frac{J_{p_1^\beta \dots p_{N_\beta}^\beta}}{N_\beta} \Big) . \tag{18}$$

The symmetry factor $S_{N_1 \dots N_B}$ is obtained as follows: If ν_i of the B numbers N_β in a given tuple $(N_1, \dots, N_B)$ are equal to i, then $S_{N_1 \dots N_B} = \prod_{i=1}^{N_B} \nu_i!$.

We stress that these weight functions $G_{|p_1^1 \dots p_{N_1}^1 | \dots | p_1^B \dots p_{N_B}^B|}$ constitute the QFT; we construct these functions rigorously and not a measure. The formal relation to the partition function gives identities (Ward + Schwinger-Dyson) between the weight functions. These identities, whenever defined, are used to extend the weight functions into regions for parameters where the measure does not exist. In the very end, QFT is understood in terms of Schwinger or Wightman functions and scattering amplitudes, not in terms of a measure.

Now comes the crucial step for the construction of the weight functions. We turn the Ward identity (17) into a formula for the second derivative $\sum_{n \in I} \frac{\partial^2 \mathcal{Z}[J]}{\partial J_{an} \partial J_{np}}$ of the partition function, thus giving new relations for $G_{\dots}$. We have to identify the kernel of multiplication by $(E_p - E_a)$. For injective $m \mapsto E_m$ this kernel is given

by $W_a[J]\delta_{ap}$ for some function $W_a[J]$. This function is identified by inserting (18) into $\sum_{n\in I} \frac{\partial^2 \exp(\log \mathcal{Z}[J])}{\partial J_{an}\partial J_{np}}$ and carefully registering the possibilities which give rise to a factor δ_{ap}. We find [18]:

Theorem 2.2

$$\sum_{n\in I} \frac{\partial^2 \mathcal{Z}[J]}{\partial J_{an}\partial J_{np}} = \delta_{ap}\Big\{V^2 \sum_{(K)} \frac{J_{P_1}\cdots J_{P_K}}{S_{(K)}} \Big(\sum_{n\in I} \frac{G_{|an|P_1|\dots|P_K|}}{V^{|K|+1}} + \frac{G_{|a|a|P_1|\dots|P_K|}}{V^{|K|+2}} + \sum_{r\geq 1} \sum_{q_1,\dots,q_r\in I} \frac{G_{|q_1 a q_1\dots q_r|P_1|\dots|P_K|} J^r_{q_1\dots q_r}}{V^{|K|+1}} \Big) + V^4 \sum_{(K),(K')} \frac{J_{P_1}\cdots J_{P_K} J_{Q_1}\cdots J_{Q_{K'}}}{S_{(K)}S_{(K')}} \frac{G_{|a|P_1|\dots|P_K|}}{V^{|K|+1}} \frac{G_{|a|Q_1|\dots|Q_{K'}|}}{V^{|K'|+1}} \Big\} \mathcal{Z}[J] + \frac{V}{E_p - E_a} \sum_{n\in I} \Big(J_{pn}\frac{\partial \mathcal{Z}[J]}{\partial J_{an}} - J_{na}\frac{\partial \mathcal{Z}[J]}{\partial J_{np}} \Big) . \tag{19}$$

Formula (19) is the core of our approach. It is a consequence of the unitary group action and the cycle structure of the partition function. The importance lies in the fact that the formula allows to kill two J-derivatives in the partition function. As we describe below, this is the key step in breaking up the tower of Schwinger-Dyson equations.

2.3 Schwinger-Dyson Equations

We can write the action as $S = \frac{V}{2}\sum_{a,b}(E_a + E_b)\Phi_{ab}\Phi_{ba} + VS_{int}[\Phi]$, where E_a are the eigenvalues of E. Functional integration yields, up to an irrelevant constant,

$$\mathcal{Z}[J] = e^{-VS_{int}[\frac{\partial}{V\partial J}]} e^{\frac{V}{2}\langle J,J\rangle_E} , \qquad \langle J,J\rangle_E := \sum_{m,n\in I} \frac{J_{mn}J_{nm}}{E_m + E_n} . \tag{20}$$

Acually, this formula is the *definition* of the partition function in any rigorous approach, and $\frac{1}{E_m+E_n}$ is the covariance. Instead of a perturbative expansion of $e^{-VS_{int}[\frac{\partial}{V\partial J}]}$ we apply those J-derivatives to (20) which give rise to a correlation function $G_{\dots}$ on the lhs. On the rhs of (20), these external derivatives combine with internal derivatives from $S_{int}[\frac{\partial}{V\partial J}]$ to certain identities for $G_{\dots}$. These Schwinger-Dyson equations are often of little use because they express an N-point function in terms of $(N+2)$-point functions. But thanks to (19) we can express the $(N+2)$-point function on the rhs in terms of N'-point functions with $N' \leq N$.

Let us look at this mechanism for the 2-point function $G_{|ab|}$ for $a \neq b$. According to (18), $G_{|ab|}$ is obtained by deriving (20) with respect to J_{ba} and J_{ab}:

$$\begin{aligned} G_{|ab|} &= \frac{1}{V\mathcal{Z}[0]} \frac{\partial^2 \mathcal{Z}[J]}{\partial J_{ba} \partial J_{ab}}\Big|_{J=0} \qquad \text{(disconnected part of } \mathcal{Z} \text{ does not contribute for } a \neq b\text{)} \\ &= \frac{1}{V\mathcal{Z}[0]} \Big\{ \frac{\partial}{\partial J_{ba}} e^{-VS_{int}\left[\frac{\partial}{V\partial J}\right]} \frac{\partial}{\partial J_{ab}} e^{\frac{V}{2}\langle J,J\rangle_E} \Big\}_{J=0} \\ &= \frac{1}{(E_a+E_b)\mathcal{Z}[0]} \Big\{ \frac{\partial}{\partial J_{ba}} e^{-VS_{int}\left[\frac{\partial}{V\partial J}\right]} J_{ba} e^{\frac{V}{2}\langle J,J\rangle_E} \Big\}_{J=0} \qquad (21) \\ &= \frac{1}{E_a+E_b} + \frac{1}{(E_a+E_b)\mathcal{Z}[0]} \Big\{ \Big(\Phi_{ab} \frac{\partial(-VS_{int})}{\partial \Phi_{ab}}\Big)\Big[\frac{\partial}{V\partial J}\Big] \Big\} \mathcal{Z}[J]\Big|_{J=0} . \end{aligned}$$

Now observe that $\frac{\partial(-VS_{int})}{\partial \Phi_{ab}}$ contains, for any polynomial interaction, the derivative $\sum_n \frac{\partial^2}{\partial J_{an}\partial J_{np}}$ which we know from (19). In case of the quartic matrix model with interaction $\frac{\lambda_4}{4}\Phi^4$ we have $\frac{\partial(-VS_{int})}{\partial \Phi_{ab}} = -\lambda_4 V \sum_{n,p\in I} \Phi_{bp}\Phi_{pn}\Phi_{na}$, hence

$$\Big(\Phi_{ab} \frac{\partial(-VS_{int})}{\partial \Phi_{ab}}\Big)\Big[\frac{\partial}{V\partial J}\Big] = -\frac{\lambda_4}{V^3} \sum_{p,n\in I} \frac{\partial^2}{\partial J_{pb}\partial J_{ba}} \frac{\partial^2}{\partial J_{an}\partial J_{np}} .$$

This is inserted into (21), then we insert (19) up to $\mathcal{O}(J^2)$. Finally one needs the expansion $\frac{\partial^2 \mathcal{Z}[J]}{\partial J_{pb}\partial J_{bp}} = (VG_{|pb|} + \delta_{pb} G_{|p|b|})\mathcal{Z}[0] + \mathcal{O}(J)$ and $\frac{\partial J_{rr}}{\partial J_{ab}} = 0$ for $a \neq b$. One arrives at [18]:

$$\left.\begin{aligned} G_{|ab|} = \frac{1}{E_a+E_b} - \frac{\lambda_4}{E_a+E_b}\frac{1}{V}\sum_{p\in I}\Big(G_{|ab|}G_{|ap|} - \frac{G_{|pb|}-G_{|ab|}}{E_p-E_a}\Big) \end{aligned}\right\} \qquad (22a)$$

$$\left.\begin{aligned} -\frac{\lambda_4}{V^2(E_a+E_b)}\Big(G_{|a|a|}G_{|ab|} + \frac{1}{V}\sum_{n\in I} G_{|an|ab|} \\ + G_{|aaab|} + G_{|baba|} - \frac{G_{|b|b|}-G_{|a|b|}}{E_b-E_a}\Big) \end{aligned}\right\} \qquad (22b)$$

$$\left.\begin{aligned} -\frac{\lambda_4}{V^4(E_a+E_b)} G_{|a|a|ab|} . \end{aligned}\right\} \qquad (22c)$$

It can be checked [18] that in a genus expansion $G_{\dots} = \sum_{g=0}^{\infty} V^{-2g} G^{(g)}_{\dots}$ (which is probably not convergent but Borel summable), precisely the line (22a) preserves the genus, the lines (22b) increase $g \mapsto g+1$ and the line (22c) increases $g \mapsto g+2$.

We will not rely on a genus expansion. Instead we consider a scaling limit $V \to \infty$ such that the densitised index summation $\frac{1}{V}\sum_{p\in I}$ remains finite. Then the exact Schwinger-Dyson equation for $G_{|ab|}$ coincides with its restriction (22a) to the planar

sector $g = 0$, a closed non-linear equation for $G^{(0)}_{|ab|}$ alone. There might exist other reasonable limits which take (22b) and (22c) into account, similar to the double scaling limit [4, 10, 13] in matrix models. Here we choose a planar limit, but even here a non-trivial topology survives: The higher boundary components $B \geq 2$ are not suppressed; and in fact these contributions from $B \geq 2$ make the model interesting!

By similar calculation we derive the Schwinger-Dyson equation for higher N-point functions. This expresses the N-point function $G_{|ab_1\dots b_{N-1}|}$ in terms of its summation

$$\frac{\lambda_4}{E_a + E_{b_1}} \frac{1}{V} \sum_{p\in I} \left(G_{|ap|} G_{|ab_1\dots b_{N-1}|} - \frac{G_{|pb_1\dots b_{N-1}|} - G_{|ab_1\dots b_{N-1}|}}{E_p - E_a} \right)$$

and several other functions [18]. It turns out that a real theory with $\Phi = \Phi^*$ admits a short-cut which directly gives the higher N-point functions without any index summation. Since the equations for $G_{\dots}$ are real and $\overline{J_{ab}} = J_{ba}$, the reality $\mathcal{Z} = \overline{\mathcal{Z}}$ implies (in addition to invariance under cyclic permutations) invariance under orientation reversal

$$G_{|p_1^1 p_2^1 \dots p_{N_1}^1 | \dots | p_1^B p_2^B \dots p_{N_B}^B|} = G_{|p_1^1 p_{N_1}^1 \dots p_2^1 | \dots | p_1^B p_{N_B}^B \dots p_2^B|} \,. \tag{23}$$

Whereas empty for $G_{|ab|}$, in $(E_a + E_{b_1}) G_{ab_1 b_2 \dots b_{N-1}} - (E_a + E_{b_{N-1}}) G_{ab_{N-1}\dots b_2 b_1}$ the identities (23) lead to many cancellations which result in a universal algebraic recursion formula [18]:

Proposition 2.3 *Given a quartic matrix model $S[\Phi] = V \operatorname{tr}(E\Phi^2 + \frac{\lambda_4}{4}\Phi^4)$ with E of compact resolvent. Then in a scaling limit $V \to \infty$ with $\frac{1}{V}\sum_{i\in I}$ finite, the $(B = 1)$-sector of $\log \mathcal{Z}$ is given by*

$$G_{|ab|} = \frac{1}{E_a + E_b} - \frac{\lambda_4}{E_a + E_b} \frac{1}{V} \sum_{p\in I} \left(G_{|ab|} G_{|ap|} - \frac{G_{|pb|} - G_{|ab|}}{E_p - E_a} \right) , \tag{24a}$$

$$G_{|b_0 b_1 \dots b_{N-1}|} \tag{24b}$$

$$= (-\lambda_4) \sum_{l=1}^{\frac{N-2}{2}} \frac{G_{|b_0 b_1 \dots b_{2l-1}|} G_{|b_{2l} b_{2l+1} \dots b_{N-1}|} - G_{|b_{2l} b_1 \dots b_{2l-1}|} G_{|b_0 b_{2l+1} \dots b_{N-1}|}}{(E_{b_0} - E_{b_{2l}})(E_{b_1} - E_{b_{N-1}})} \,.$$

The self-consistency equation (24a) was first obtained in [19] for the Moyal model by the graphical method proposed by [9]. There we also solved the renormalisation problem resulting from the divergent summation $\sum_{p\in I}$. The non-linearity of (24a) was a considerable challenge which we successfully addressed in [18, 21].

The other topological sectors $B \geq 2$ made of $(N_1 + \dots + N_B)$-point functions $G_{|b_1^1 \dots b_{N_1}^1 | \dots | b_1^1 \dots b_{N_B}^B|}$ are similar in the following sense [18]: The basic functions with all $N_i \leq 2$ satisfy an equation with index summation as (24a), but in contrast to the

2-point function these equations are linear. The other functions with one $N_i \geq 3$ are purely algebraic.

We make the following key observation: An affine transformation $E \mapsto ZE + C$ together with a corresponding rescaling $\lambda_4 \mapsto Z^2\lambda_4$ leaves the algebraic equations invariant:

Theorem 2.4 *Given a real quartic matrix model with* $S = V\,\mathrm{tr}(E\Phi^2 + \frac{\lambda_4}{4}\Phi^4)$ *and* $m \mapsto E_m$ *injective, which determines the set* $G_{|p^1_1 \ldots p^1_{N_1}|\ldots|p^B_1 \ldots p^B_{N_B}|}$ *of* $(N_1 + \ldots + N_B)$*-point functions. Assume that the basic functions with all* $N_i \leq 2$ *are turned finite by* $E_a \mapsto Z(E_a + \frac{\mu^2}{2} - \frac{\mu^2_{bare}}{2})$ *and* $\lambda_4 \mapsto Z^2\lambda_4$*. Then all functions with one* $N_i \geq 3$

1. *are finite without further need of a renormalisation of* λ*, i.e. all renormalisable quartic matrix models have vanishing* β*-function,*
2. *are given by universal algebraic recursion formulae in terms of renormalised basic functions with* $N_i \leq 2$*.*

The theorem tells us that vanishing of the β-function for the self-dual Φ^4_4-model on Moyal space (proved in [9] to all orders in perturbation theory) is generic to all quartic matrix models, and the result even holds non-perturbatively!

We remark that the algebraic equations for $N_i \geq 3$ have a graphical realisation in terms of non-crossing chord diagrams with additional decoration which describe the denominators $\frac{1}{E_{b_i} - E_{b_j}}$. The different chord structures are counted by the Catalan numbers. These functions alone would make the higher N-point functions very close to trivial. It is the inclusion of the $(2+2+\ldots+2)$-point functions which gives a rich structure.

2.4 Infinite Volume Limit and Renormalisation

We return to the Moyal-space regularisation of the $\lambda\phi^4_4$-model. We know that the *unrenormalised* 2-point function $G_{|\underline{a}\underline{b}|}$ satisfies the self-consistency equation (24a) for $E_{\underline{m}} = Z\Big(\frac{|\underline{m}|}{\sqrt{V}} + \frac{\mu^2_{bare}}{2}\Big)$ and $\lambda_4 = Z^2\lambda$. Because of the vanishing β-function (Theorem 2.4), there is no need to introduce a bare coupling λ_{bare}. The matrix indices have ranges $\underline{a}, \cdots \in I := \mathbb{N}^2_{\mathcal{N}}$, i.e. pairs of natural numbers with certain cut-off. The index sum diverges for $\mathbb{N}^2_{\mathcal{N}} \mapsto \mathbb{N}^2$.

It is important that all functions only depend on the spectrum of $E_{\underline{m}}$, i.e. on the norms $|\underline{m}| = m_1 + m_2$ and not on m_1, m_2 separately. It turns out that also renormalisation respects this degeneracy. Therefore, all index sums reduce to $\sum_{\underline{p} \in \mathbb{N}^2_{\mathcal{N}}} f(|\underline{p}|) = \sum_{|\underline{p}|=0}^{\mathcal{N}} (|\underline{p}|+1) f(|\underline{p}|)$. The Eqs. (24a) result from (22) in a scaling limit $V \to \infty$ and $\frac{1}{V}\sum_{|\underline{p}|=0}^{\mathcal{N}} (|\underline{p}|+1) f(|\underline{p}|)$ finite. The most natural way to achieve this is to keep the ratio $\frac{\mathcal{N}}{\sqrt{V\mu^4}} = \Lambda^2(1+\mathcal{Y})$ fixed. Note that $V = \big(\frac{\theta}{4}\big)^2 \to \infty$ is a limit of extreme noncommutativity! The new parameter $(1+\mathcal{Y})$ corresponds to a finite wavefunction renormalisation, identified later to decouple our equations, and

μ will be the renormalised mass. The parameter Λ^2 represents an ultraviolet cut-off which is sent to $\Lambda \to \infty$ in the very end (continuum limit). In the scaling limit, functions of $\frac{|p|}{\sqrt{V}} =: \mu^2(1+\mathcal{Y})p$ converge to functions of 'continuous matrix indices' $p \in [0, \Lambda^2]$, and the densitised index summation converges to a Riemann integral. After all these steps, the unrenormalised function $G^{(ur)}_{ab} := \lim_{V\to\infty} \mu^2 G_{|\underline{ab}|}$ satisfies the following equation resulting from (24a):

$$G^{(ur)}_{ab} = \frac{1}{Z\big(\frac{\mu^2_{bare}}{\mu^2} + (a+b)(1+\mathcal{Y})\big)} - \frac{Z^2\lambda(1+\mathcal{Y})^2}{Z\big(\frac{\mu^2_{bare}}{\mu^2} + (a+b)(1+\mathcal{Y})\big)} \int_0^{\Lambda^2} pdp \left(G^{(ur)}_{ab} G^{(ur)}_{ap} - \frac{G^{(ur)}_{pb} - G^{(ur)}_{ab}}{(1+\mathcal{Y})Z(p-a)} \right) . \tag{25}$$

The next step is the renormalisation which constructs the limit $\Lambda^2 \to \infty$. We pass to the 1PI function defined by

$$\big(G^{(ur)}_{ab}\big)^{-1} =: Z\big(\frac{\mu^2_{bare}}{\mu^2} + (a+b)(1+\mathcal{Y})\big) - \Gamma^{(ur)}_{ab} . \tag{26a}$$

We *define* the renormalised 1PI function Γ_{ab} via second-order Taylor formula with remainder

$$\Gamma^{(ur)}_{ab} = Z\frac{\mu^2_{bare}}{\mu^2} - 1 + (Z-1)(a+b)(1+\mathcal{Y}) - \Gamma_{ab} ,$$
$$\Gamma_{00} := 0 , \quad (\partial\Gamma)_{00} := 0 \tag{26b}$$

and then the renormalised connected function G_{ab} as

$$\big(G_{ab}\big)^{-1} = 1 + (a+b)(1+\mathcal{Y}) - \Gamma_{ab} .$$

We stress that this procedure would be completely wrong for other models. Renormalisation is a recursive procedure [3, 24, 47] which has to take subdivergences into account. Of course our 4-point subfunctions diverge, but these divergences are exactly cancelled by the divergent vertex factors $(-Z^2\lambda)$ because β is zero. So there only remain divergent 2-point subfunctions, but inductively they are already renormalised. In conclusion, $\beta = 0$ permits a non-perturbative renormalisation prescription, in some sense a renormalisation of all Feynman graphs at once. In detail, we view (25) via (26) as an equation for Γ_{ab} and have together with $\Gamma_{00} = 0$ and $(\partial\Gamma)_{00} = 0$ three equations for the three functions Γ_{ab}, $\frac{\mu_{bare}}{\mu}$ and Z which allows us to eliminate μ_{bare} and Z.

Eliminating μ_{bare} is easy; eliminating Z is difficult due to the non-linearity in (25). We propose the following trick which postpones the non-linearity: If we multiply (25) by $Z\big(\frac{\mu_{bare}^2}{\mu^2} + (a+b)(1+\mathcal{Y})\big)\big/G_{ab}^{(ur)}$, then the previously non-linear term is independent of b. So we subtract from that equation the equation at $b = 0$. Our problem is then equivalent to the difference equation plus (25) at $b = 0$. The difference equation reads after elimination of μ_{bare}, but before elimination of Z,

$$\frac{Z^{-1}}{(1+\mathcal{Y})}\Big(\frac{1}{G_{ab}} - \frac{1}{G_{a0}}\Big) = b - \lambda\int_0^{\Lambda^2} p\,dp\;\frac{\frac{G_{pb}}{G_{ab}} - \frac{G_{p0}}{G_{a0}}}{p-a}\;. \tag{27}$$

Differentiation $\frac{d}{db}\big|_{a=b=0}$ of (27) yields Z^{-1} in terms of G_{ab} and its derivative. The resulting derivative G' can be avoided by adjusting $\mathcal{Y} := -\lambda\lim\limits_{b\to0}\int_0^{\Lambda^2} dp\;\frac{G_{pb}-G_{p0}}{b}$. This choice leads to $\frac{Z^{-1}}{(1+\mathcal{Y})} = 1 - \lambda\int_0^{\Lambda^2} dp\;\; G_{p0}$, which is a perturbatively divergent integral for $\Lambda\to\infty$. Inserting Z^{-1} and $\mathcal{Y}$ back into (27) we end up in a *linear* integral equation for the difference function $D_{ab} := \frac{a}{b}(G_{ab} - G_{a0})$ to the boundary. The non-linearity restricts to the boundary function G_{a0} where the second index is put to zero. Assuming $a\mapsto G_{ab}$ Hölder-continuous, we can pass to Cauchy principal values. In terms of the *finite Hilbert transform*

$$\mathcal{H}_a^\Lambda[f(\bullet)] := \frac{1}{\pi}\lim_{\epsilon\to0}\Big(\int_0^{a-\epsilon} + \int_{a+\epsilon}^{\Lambda^2}\Big)\frac{f(q)\,dq}{q-a}\;, \tag{28}$$

the integral equation becomes

$$\Big(\frac{b}{a} + \frac{1+\lambda\pi a\mathcal{H}_a^\Lambda\big[G_{\bullet0}\big]}{aG_{a0}}\Big)D_{ab} - \lambda\pi\mathcal{H}_a^\Lambda\big[D_{\bullet b}\big] = -G_{a0}\;. \tag{29}$$

Equation (29) is a well-known singular integral equation of Carleman type [5, 41]:

Theorem 2.5 ([41], transformed from $[-1,1]$ to $[0,\Lambda^2]$) *The singular linear integral equation*

$$h(a)y(a) - \lambda\pi\mathcal{H}_a^\Lambda[y] = f(a)\;,\qquad a\in\,]0,\Lambda^2[\;,$$

is for $h(a)$ continuous on $]0,\Lambda^2[$, Hölder-continuous near $0,\Lambda^2$, and $f\in L^p$ for some $p>1$ (determined by $\vartheta(0)$ and $\vartheta(\Lambda^2)$) solved by

$$y(a) = \frac{\sin(\vartheta(a))e^{-\mathcal{H}_a^\Lambda[\pi-\vartheta]}}{\lambda\pi a}\Big(af(a)e^{\mathcal{H}_a^\Lambda[\pi-\vartheta]}\cos(\vartheta(a)) + \mathcal{H}_a^\Lambda\Big[e^{\mathcal{H}_\bullet^\Lambda[\pi-\vartheta]}\bullet f(\bullet)\sin(\vartheta(\bullet))\Big] + C\Big) \tag{30a}$$

$$\stackrel{*}{=} \frac{\sin(\vartheta(a))e^{\mathcal{H}_a^\Lambda[\vartheta]}}{\lambda\pi}\Big(f(a)e^{-\mathcal{H}_a^\Lambda[\vartheta]}\cos(\vartheta(a)) + \mathcal{H}_a^\Lambda\Big[e^{-\mathcal{H}_\bullet^\Lambda[\vartheta]}f(\bullet)\sin(\vartheta(\bullet))\Big] + \frac{C'}{\Lambda^2-a}\Big)\,, \tag{30b}$$

where $\vartheta(a) = \underset{[0,\pi]}{\arctan}\left(\frac{\lambda\pi}{h(a)}\right)$ *and* C, C' *are arbitrary constants.*

The possibility of $C, C' \neq 0$ is due to the fact that the finite Hilbert transform has a kernel, in contrast to the infinite Hilbert transform with integration over $\mathbb{R}$. The two formulae (30a) and (30b) are formally equivalent, but the solutions belong to different function classes and normalisation conditions may (and will) make a choice.

A lengthy discussion [21] shows that such a constant C, C' arises for $\lambda > 0$ but not for $\lambda < 0$. The key step in this analysis is to regard the defining equation for ϑ as a Carleman type singular integral equation for G_{a0}. This allows to express G_{a0} in terms of ϑ, and various identities in [41] and trigonometric addition theorems give the result:

Theorem 2.6 ([21]) *The matrix 2-point function* G_{ab} *of the* $\lambda\phi_4^{\star 4}$*-model is in infinite volume limit given in terms of the boundary 2-point function* G_{0a} *by the equation*

$$G_{ab} = \frac{\sin(\tau_b(a))}{|\lambda|\pi a}\mathrm{e}^{\mathrm{sign}(\lambda)(\mathcal{H}_0^\Lambda[\tau_0(\bullet)]-\mathcal{H}_a^\Lambda[\tau_b(\bullet)])} \times \begin{cases} 1 & \text{for } \lambda < 0 \\ \left(1+\frac{Ca+bF(b)}{\Lambda^2-a}\right) & \text{for } \lambda > 0\,, \end{cases} \tag{31}$$

$$\tau_b(a) := \underset{[0,\pi]}{\arctan}\left(\frac{|\lambda|\pi a}{b + \frac{1+\lambda\pi a\mathcal{H}_a^\Lambda[G_{\bullet 0}]}{G_{a0}}}\right), \tag{32}$$

where C *is a undetermined constant and* $bF(b)$ *an undetermined function of* b *vanishing at* $b = 0$.

Some remarks:

- We proved this theorem in 2012 for $\lambda > 0$ under the assumption $C' = 0$ in (30b), but knew that non-trivial solutions of the homogeneous Carleman equation parametrised by $C' \neq 0$ are possible. That no such term arises for $\lambda < 0$ (if angles are redefined $\vartheta \mapsto \tau$) is a recent result [21].
- We expect C, F to be Λ-dependent so that $\left(1+\frac{Ca+bF(b)}{\Lambda^2-a}\right) \overset{\Lambda\to\infty}{\longrightarrow} 1+\tilde{C}a + b\tilde{F}(b)$.
- An important observation is $G_{ab} \geq 0$, at least for $\lambda < 0$. This is a truly non-perturbative result; individual Feynman graphs show no positivity at all!

- As in [19], the equation for G_{ab} can be solved perturbatively. This reproduces exactly [18] the Feynman graph calculation! Matching at $\lambda = 0$ requires C, F to be flat functions of λ (all derivatives vanish at zero).
- Because of $\mathcal{H}_a^\Lambda[G_{\bullet 0}] \overset{a\to\Lambda^2}{\longrightarrow} -\infty$, the naïve arctan series is dangerous for $\lambda > 0$. Unless there are cancellations, we expect zero radius of convergence!
- From (31) we deduce the finite wavefunction renormalisation

$$\mathcal{Y} := -1 - \frac{dG_{ab}}{db}\Big|_{a=b=0} = \int_0^{\Lambda^2} \frac{dp}{(\lambda\pi p)^2 + \left(\frac{1+\lambda\pi p\mathcal{H}_p^\Lambda[G_{\bullet 0}]}{G_{p0}}\right)^2} - \begin{cases} 0 & \text{for } \lambda < 0\,, \\ F(0) & \text{for } \lambda > 0\,. \end{cases} \tag{33}$$

- The partition function $\mathcal{Z}$ is undefined for $\lambda < 0$. But the Schwinger-Dyson equations for G_{ab} and for higher functions, and with them $\log \mathcal{Z}$, extend to $\lambda < 0$. These extensions are unique but probably not analytic in a neighbourhood of $\lambda = 0$.

It remains to identify the boundary function G_{a0}. It is determined by (25) at $b = 0$. The equation involves subtle cancellations which so far we did not succeed to control. As substitute we use a symmetry argument. Given the boundary function G_{a0}, the Carleman theory computes the full 2-point function G_{ab} via (31). In particular, we get G_{0b} as function of G_{a0}. But the 2-point function is symmetric, $G_{ab} = G_{ba}$, and the special case $a = 0$ leads to the following self-consistency equation:

Proposition 2.7 *The limit $\theta \to \infty$ of $\lambda\phi_4^4$-theory on Moyal space is for $\lambda \le 0$ determined by the solution of the fixed point equation $G = TG$,*

$$G_{b0} \equiv G_{0b} = \frac{1}{1+b} \exp\left(-\lambda \int_0^b dt \int_0^{\Lambda^2} \frac{dp}{(\lambda\pi p)^2 + \left(t + \frac{1+\lambda\pi p\mathcal{H}_p^\Lambda[G_{\bullet 0}]}{G_{p0}}\right)^2}\right). \tag{34}$$

At this point we can eventually send $\Lambda \to \infty$. Any solution of (34) is automatically smooth and monotonously decreasing. Any solution of the true equation (25) (without the difference to $b = 0$) also solves the master equation (34), but not necessarily conversely. In case of a unique solution of (34), it is enough to check one candidate. Existence of a solution of (34) is established by the Schauder fixed point theorem. This was done in [18] for $\lambda > 0$, and is work in progress for $\lambda < 0$.

This solution provides G_{ab} via (31) and all higher correlation functions via the universal algebraic recursion formulae (24b), or via the linear equations for the basic $(N_1 + \ldots + N_B)$-point functions [18].

3 Schwinger Functions and Reflection Positivity

3.1 Reverting the Matrix Representation

In the previous section we have constructed the connected matrix correlation functions $G_{|\underline{q}_1^1 \dots \underline{q}_{N_1}^1| \dots |\underline{q}_1^B \dots \underline{q}_{N_B}^B|}$ of the $(\theta \to \infty)$-limit of $\lambda\phi_4^4$-theory on Moyal space. These functions arise from the topological expansion (18) of the free energy. Now we revert the introduction of the matrix basis (4) to obtain Schwinger functions [39] in position space:

$$S_c(\mu x_1, \dots, \mu x_N) := \lim_{V\mu^4 \to \infty} \lim_{\Lambda \to \infty} \frac{1}{64\pi^2} \sum_{N_1 + \dots + N_B = N} \sum_{\underline{q}_i^\beta \in \mathbb{N}^2_{\mathcal{N}}} G_{|\underline{q}_1^1 \dots \underline{q}_{N_1}^1| \dots |\underline{q}_1^B \dots \underline{q}_{N_B}^B|}$$

$$\times \sum_{\sigma \in \mathcal{S}_N} \prod_{\beta=1}^{B} \frac{f_{\underline{q}_1 \underline{q}_2}(x_{\sigma(s_\beta+1)}) \cdots f_{\underline{q}_{N_\beta} \underline{q}_1}(x_{\sigma(s_\beta+N_\beta)})}{V\mu^4 N_\beta} , \tag{35}$$

where $s_\beta := N_1 + \dots + N_{\beta-1}$ and $\mathcal{N} = \Lambda^2(1+\Upsilon)\sqrt{V\mu^4}$. The $G_{\dots}$ are made dimensionless by appropriate rescaling in μ. These Schwinger functions are fully symmetric in $\mu x_1, \dots, \mu x_N$. We recall that the prefactor of $G_{\dots}$ in (18) was V^{2-B}. The factor V^{-B} is distributed over the B cycles. We have thus defined the density as $V^{-2} \log \frac{\mathcal{Z}[J]}{\mathcal{Z}[0]}$ in agreement with the spectral geometry of the Moyal plane with harmonic propagation [11]. There is one delicate point with this definition: We perform the limits $\lim_{V\mu^4 \to \infty}, \lim_{\Lambda \to \infty}$ in different order than before and leave the justification as an open problem.

The next step consists in representing $G_{\dots|\underline{p}_1 \dots \underline{p}_{N_\beta}|\dots}$, for every boundary component, as a Laplace transform in $\frac{1}{\sqrt{V\mu^4}}(|\underline{p}_1| + \dots + |\underline{p}_{N_\beta}|)$ and Fourier transform in $\frac{1}{\sqrt{V\mu^4}}(|\underline{p}_{i+1}| - |\underline{p}_i|)$. For example,

$$G_{|\underline{a}\underline{b}|} = \int_0^\infty dt \int_{-\infty}^{\infty} d\omega \; \mathcal{G}(t,\omega) e^{-\frac{t}{\sqrt{V\mu^4}}(|a|+|b|) - \mathrm{i}\frac{\omega}{\sqrt{V\mu^4}}(|a|-|b|)} . \tag{36}$$

Compatibility with the infinite volume limit to continuous matrix indices $\frac{|a|}{\sqrt{V\mu^4}} \to (1+\Upsilon)a$ is assumed.

The f_{mn} are products of associated Laguerre polynomials with a Gaußian [12, 20]. The summation over the matrix indices is performed (at finite volume V) with the

help of generating functions for the Laguerre polynomials. In two dimensions one has [20]:

$$\sum_{m_1,\dots,m_L=0}^{\infty} \frac{1}{\theta}\prod_{i=1}^{L} f_{m_i m_{i+1}}(x_i) z_i^{m_i}$$
$$= \frac{2^L}{\theta(1-\prod_{i=1}^{L}(-z_i))} \exp\left(-\frac{\sum_{i=1}^{L}\|x_i\|^2}{\theta}\frac{1+\prod_{i=1}^{L}(-z_i)}{1-\prod_{i=1}^{L}(-z_i)}\right)$$
$$\times \exp\left(-\frac{2}{\theta}\sum_{1\le k<l\le L}\Big(\big(\langle x_k, x_l\rangle - \mathrm{i}x_k\times x_l\big)\frac{\prod_{j=k+1}^{l}(-z_j)}{1-\prod_{i=1}^{L}(-z_i)}\right.$$
$$\left. + \big(\langle x_k, x_l\rangle + \mathrm{i}x_k\times x_l\big)\frac{\prod_{j=l+1}^{L+k}(-z_j)}{1-\prod_{i=1}^{L}(-z_i)}\Big)\right). \tag{37}$$

The z_i are of the form $z \sim \exp(-\frac{t+\mathrm{i}\omega}{\sqrt{V\mu^4}})$ as in (36). At this point the limit $V\mu^4 = \frac{\mu^2\theta^2}{16} \to \infty$ can be taken where z_i converges to 1. Thus for odd L the limit is zero, whereas for L even one has $\lim_{\theta\to\infty}\theta(1-\prod_{i=1}^{L}(-z_i)) = \frac{4Lt}{\mu^2}$. The vector product and all Fourier variables ω drop out, and the scalar products (37) arrange with the norms to $\mu^2\|x_1 - x_2 + \cdots - x_L\|^2$. Absence of the Fourier variables means that all matrix indices per boundary component are equal. The Laplace transform is easily reverted after introduction of an auxiliary p-integration per boundary component. The final result is:

Theorem 3.1 *The connected N-point Schwinger functions of the $\lambda\phi_4^4$-model on extreme Moyal space $\theta \to \infty$ are given by*

$$S_c(\mu x_1, \dots, \mu x_N)$$
$$= \frac{1}{64\pi^2}\sum_{\substack{N_1+\dots+N_B=N\\ N_\beta \text{ even}}}\sum_{\sigma\in\mathcal{S}_N}\left(\prod_{\beta=1}^{B}\frac{4^{N_\beta}}{N_\beta}\int_{\mathbb{R}^4}\frac{dp_\beta}{4\pi^2\mu^4}\, e^{\mathrm{i}\left\langle \frac{p_\beta}{\mu}, \sum_{i=1}^{N_\beta}(-1)^{i-1}\mu x_{\sigma(s_\beta+i)}\right\rangle}\right)$$
$$\times G_{\underbrace{\frac{\|p_1\|^2}{2\mu^2(1+\Upsilon)},\dots,\frac{\|p_1\|^2}{2\mu^2(1+\Upsilon)}}_{N_1}|\dots|\underbrace{\frac{\|p_B\|^2}{2\mu^2(1+\Upsilon)},\dots,\frac{\|p_B\|^2}{2\mu^2(1+\Upsilon)}}_{N_B}}. \tag{38}$$

Some comments:

- Only a restricted sector of the underlying matrix model contributes to position space: All strands of the same boundary component carry the same matrix index.
- Schwinger functions are symmetric and invariant under the full Euclidean group. This comes truly surprising since $\theta \neq 0$ breaks both translation invariance and

manifest rotation invariance. The limit $\theta \to \infty$ was expected to make this symmetry violation even worse!

- The most interesting sector is the case where every boundary component has $N_\beta = 2$ indices. It is described by the $(2+\ldots+2)$-point functions $G_{\frac{\|p_1\|^2}{2\mu^2(1+\Upsilon)}\frac{\|p_1\|^2}{2\mu^2(1+\Upsilon)}\left|\ldots\right|\frac{\|p_B\|^2}{2\mu^2(1+\Upsilon)}\frac{\|p_B\|^2}{2\mu^2(1+\Upsilon)}}$. The corresponding matrix functions $G_{a_1 a_1|\ldots|a_B a_B}$ satisfy more complicated singular (but linear!) integral equations. The solution techniques of the Carleman problem can be used in a first step to regularise these equations to linear integral equations of Fredholm type. These have always a unique solution for $|\lambda|$ small enough.
- This $(2+\ldots+2)$-sector describes the propagation and interaction of B (at the moment Euclidean) particles without any momentum exchange. Such a behaviour is necessary in any integrable model [27, 32]. It is tempting to speculate that there might be an integrable structure behind that is responsible for the model being solvable and for absence of momentum transfer.
- We are aware of the problem that the absence of momentum transfer in four dimensions is a sign of *triviality*. Typical triviality proofs rely on clustering, analyticity in Mandelstam representation or absence of bound states. All this needs verification.
- That the $\theta \to \infty$ limit is so close to an ordinary field theory expected for $\theta \to 0$ can be seen from the following observation: The interaction term in momentum space

$$\frac{\lambda}{4}\int_{(\mathbb{R}^4)^4}\Big(\prod_{i=1}^{4}\frac{dp_i}{(2\pi)^4}\Big)\,\delta(p_1+\cdots+p_4)\,\exp\Big(\mathrm{i}\sum_{i<j}\langle p_i,\Theta p_j\rangle\Big)\prod_{i=1}^{4}\hat{\phi}(p_i)$$

leads to the Feynman rule $\lambda \exp\big(\mathrm{i}\sum_{i<j}\langle p_i,\Theta p_j\rangle\big)$, plus momentum conservation. For $\theta \to \infty$, this converges to zero almost everywhere by the Riemann-Lebesgue lemma, *unless* p_i, p_j *are linearly dependent*. This case of linearly dependent momenta might be protected for topological reasons, and these are precisely the boundary components $B > 1$ which guarantee full Lebesgue measure!

3.2 Osterwalder-Schrader Axioms

Under conditions identified by Osterwalder-Schrader [33, 34], Schwinger functions of a Eulidean quantum field theory permit an analytical continuation to Wightman functions [40, 45] of a true relativistic quantum field theory. In simplified terms, the reconstruction theorem of Osterwalder-Schrader for a field theory on $\mathbb{R}^D$ says:

Theorem 3.2 ([33, 34]) *Assume the Schwinger functions $S(x_1,\ldots,x_N)$ satisfy*

(OS0) factorial growth,
(OS1) Euclidean invariance,

(OS2) reflection positivity,[1]
(OS3) permutation symmetry.

Then the $S(\xi_1, \dots \xi_{N-1})\big|_{\xi_i^0>0}$, *with* $\xi_i = x_i - x_{i+1}$, *are Laplace-Fourier transforms of Wightman functions in a relativistic quantum field theory. If in addition the* $S(x_1, \dots, x_N)$ *satisfy*

(OS4) clustering

then the Wightman functions satisfy clustering, too.

The Schwinger functions (38) clearly satisfy (OS1) + (OS3). Clustering (OS4) is not realised. Bounds on $S_c(\mu x_1, \dots, \mu x_N)$ for large N follow from bounds on (24b) at coinciding indices and eventually from bounds on derivatives of the 2-point function. Formulae for $\frac{\partial^{n+\ell} G_{ab}}{\partial a^n\, \partial b^\ell}$ were derived in [21] and one has indeed a bound $\leq C(n+\ell-1)!$.

Thus the remaining problem is (OS2) reflection positivity. We will not discuss the axiom itself. Instead we rely on the Källén-Lehmann spectral representation [25, 29] of a Wightman 2-point function according to which the Wightman 2-point function is a superposition of free fields with certain mass spectrum. Wightman functions always have an analytic continuation to Schwinger functions. Comparing with $S_c(\mu\xi, 0)$ we find that the *diagonal matrix 2-point function is a Stieltjes function*, i.e. a function from $\mathbb{R}_+$ to $\mathbb{R}_+$ of the form

$$G_{aa} = \int_0^\infty \frac{d(\rho(t))}{a+t}\ , \tag{39}$$

where ρ is a positive measure. Indeed, using the residue theorem it is straightforward to check

$$S_c(\mu\xi, 0)\big|_{\xi^0>0} = \int_0^\infty \frac{2(1+\mathcal{Y})\, d\rho(t)}{\mu^4} \int_0^\infty dq^0 \int_{\mathbb{R}^3} d\vec{q}\ \hat{W}_t(q) e^{-q^0\xi^0 + i\vec{q}\cdot\vec{\xi}}\ , \tag{40}$$

$$\hat{W}_t(q) := \frac{\theta(q^0)}{(2\pi)^3}\delta\Big(\frac{(q^0)^2 - \vec{q}^2 - 2\mu^2(1+\mathcal{Y})t}{\mu^2}\Big)\ .$$

Stieltjes functions form an important subclass of the class of completely monotonic functions. We refer to [2] for an overview about completely monotonic functions and their relations to other important classes of functions. The Stieltjes integral (39) provides a unique analytic continuation of a Stieltjes function to the

[1] For each assignment $N \mapsto f_N \in \mathcal{S}^N$ of test functions, one has

$$\sum_{M,N} \int dx\, dy\ S(x_1, \dots, x_N, y_1, \dots, y_M) \overline{f_N(x_1^r, \dots, x_N^r)} f_M(y_1, \dots, y_M) \geq 0\ ,$$

where $(x^0, x^1, \dots x^{D-1})^r := (-x^0, x^1, \dots x^{D-1})$.

cut plane $\mathbb{C} \setminus]-\infty, 0[$. But the difficulty is to decide whether or not a given function is Stieltjes. Widder found criteria [44] for the real function alone which guarantee the existence of the measure and gave a sequence which weakly converges to the measure. If the extension to the complex plane is known, then a function $f : \mathbb{C} \setminus]-\infty, 0] \to \mathbb{C}$ is Stieltjes if [2]

1. $f(x) \geq 0$ for $x > 0$ (Euclidean positivity),
2. f is holomorphic on $\mathbb{C} \setminus]-\infty, 0]$,
3. f is anti-Herglotz, i.e. $\mathrm{Im}(f(x + \mathrm{i}y) \leq 0$ for $y > 0$ (Minkowskian positivity).

There is a complex inversion formula already due to Stieltjes (see [44]) which recovers the measure from the boundary values at both sides of the cut.

From the anti-Herglotz property one concludes that $p^2 \mapsto f(p^2) = \frac{1}{(p^2+\mu^2)^{1-\frac{\eta}{2}}}$ is Stieltjes precisely for $0 \leq \eta \leq 2$, i.e. slower decay than p^{-2}. In this sense, renormalisation (good decay of the propagator) contradicts positivity, and the only chance to construct a renormalisable theory in 4 dimensions is by continuation of a theory with good decay beyond its domain of definition, here to negative λ. Fourier transform implies $G(x - y) \sim \frac{e^{-\mu|x-y|}}{|x-y|^{4-(2-\eta)}}$ so that η is the anomalous dimension, which must be positive. What happens is that the *bare* anomalous dimension is positive for positive λ, but the leading term diverges. Renormalisation oversubtracts so that the renormalised anomalous dimension gets the opposite sign of λ.

3.3 Recent Numerical and Analytical Results

A first hint about the two-point function and reflection positivity can be obtained from a numerical solution of the fixed point equation (34). This was done in [21] using *Mathematica*^{TM}. The idea is to approximate G_{0b} as a piecewise linear function on $[0, \Lambda^2]$ sampled according to a geometric progression and view (34) as iteration $G_{0b}^{i+1} = (TG^i)_{0b}$ for some initial function G^0. We confirmed the convergence of this iteration in Lipschitz norm for any $\lambda \in \mathbb{R}$. It turned out that the required symmetry $G_{ab} = G_{ba}$ does not hold for $\lambda > 0$, which is a clear hint that the winding number contributions $C, F(b)$ are present for $\lambda > 0$. For $\lambda < 0$ everything is consistent within small numerical errors. This allows us to compute for $\lambda < 0$ all quantities of the model with sufficient precision.

We find clear evidence for a second-order phase transition at $\lambda_c \approx -0.39$, which is a common critical value in several independent problems. The first one is the derivative $1 + \mathcal{Y} := -\frac{dG_{0b}}{db}\big|_{b=0}$, viewed as function of λ (Fig. 1). More precisely, for $\lambda < \lambda_c$ we have $G_{0b} = 1$ in a whole neighbourhood of $b = 0$, and the length of this neighbourhood serves as an order parameter. Since also $1 + \mathcal{Y} = 0$ for $\lambda < \lambda_c$, the infinite volume limit is ill-defined; i.e. the model is inconsistent beyond λ_c. Another phase transition occurs at $\lambda = 0$. It is not visible in G_{0b} but in the full 2-point function G_{ab} which looses its symmetry for $\lambda > 0$. This means that the 'good' phase is $\lambda_c < \lambda \leq 0$.

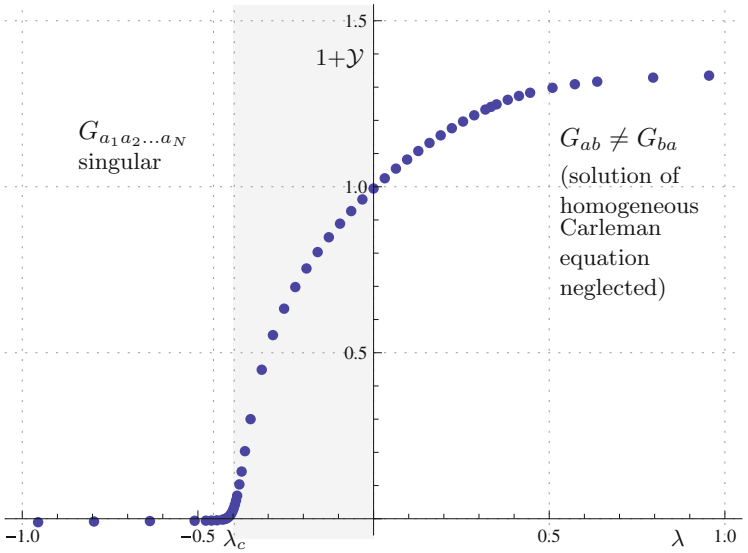


Fig. 1 $1+\mathcal{Y} := -\frac{dG_{0b}}{db}\big|_{b=0}$ as function of λ, based on G_{0b} computed for $\Lambda^2{=}10^7$ with $L = 2000$ sample points

Of paramount importance is the question whether or not $a \mapsto G_{aa}$ is a Stieltjes function. We cannot expect a definite answer from a numerical simulation because a discrete approximation, here a piecewise linear function, cannot be analytic. The criteria for complete monotonicity [2] and Widder's criterium for the Stieltjes property [44] must fail for some order n. But refining the approximation, i.e. increasing the number L of sample points, the failure should occur at larger n, with no failure in the limit. This is precisely what we observe: The critical index where complete monotonicity or Stieltjes property fails increases with the resolution, but this increase slows down for larger $|\lambda|$ and stops at precisely the same value $\lambda_c \approx -0.39$ that located the discontinuity in Fig. 1! We find clear evidence for

- a mass gap $\rho(t) = 0$ for $0 \le t < \frac{m_0^2}{\mu^2}$,
- absence of a further mass gap, i.e. scattering right away from m_0^2 and not only from the two-particle threshold on.

This provided enough motivation for an analytic treatment of the question. In a work in progress, we view (34) as a fixed point problem for $\log G_{b0} = T(\log G_{\bullet 0})(b)$, identify a Banach space $(X, \|\ \|)$ and a closed convex subset $\mathcal{K}_\lambda \subseteq X$ with the following properties for $-\frac{1}{6} \le \lambda \le 0$:

1. T maps $\mathcal{K}_\lambda$ into itself.
2. $\|Tf - Tg\| \le (1 + \frac{1}{e} + \mathcal{O}(|\lambda|))\|f - g\|$ for any $f, g \in \mathcal{K}_\lambda$.
3. $T\mathcal{K}_\lambda$ is $\|\ \|$-compact in $\mathcal{K}_\lambda$ when restricted to $[0, \Lambda^2]$.

Property 2 excludes the Banach fixed point theorem, but together with Property 3, the Schauder fixed point theorem guarantees existence of a solution G_{b0}.

As by-product of these investigations we obtain an analytic continuation of G_{z0} to the complex plane. We prove that any function in $\exp(T\mathcal{K}_\lambda)$, in particular any fixed point of (34), is anti-Herglotz. The function G_{z0} is holomorphic outside the negative reals and outside a certain curve in left half-plane. If we could prove that G_{z0} is differentiable on that curve, then G_{b0} would be a Stieltjes. From here it is still some work to prove that G_{aa} is Stieltjes, but the compatibilities established so far are an extremely encouraging sign that this should also be true. We are thus convinced that the model will define a true relativistic quantum field theory in four dimensions.

Acknowledgements We would like to cordially thank Jürgen Tolksdorf and Felix Finster for invitation to *Quantum Mathematical Physics* and hospitality during the conference in Regensburg. We submit our best wishes to Eberhard Zeidler.

References

1. G. Benfatto, V. Mastropietro, Ward identities and vanishing of the beta function for d = 1 interacting Fermi systems. J. Stat. Phys. **115**, 143–184 (2004)
2. C. Berg, Stieltjes-Pick-Bernstein-Schoenberg and their connection to complete monotonicity, in *Positive Definite Functions. From Schoenberg to Space-Time Challenges*, ed. by J. Mateu, E. Porcu (Department of Mathematics, University Jaume I, Castellon, 2008)
3. N.N. Bogolyubov, D.V. Shirkov, *Introduction to the Theory of Quantized Fields*. Interscience Monographs in Physics and Astronomy, vol. 3 (Interscience Publishers, New York, 1959)
4. E. Brezin, V.A. Kazakov, Exactly solvable field theories of closed strings. Phys. Lett. B **236**, 144–150 (1990)
5. T. Carleman, Sur la résolution de certaines équations intégrales. Arkiv for Mat., Astron. och Fysik **16**, 19pp (1922)
6. I. Chepelev, R. Roiban, Renormalization of quantum field theories on noncommutative $\mathbb{R}^d$. 1. Scalars. JHEP **0005**, 037 (2000). [hep-th/9911098]
7. I. Chepelev, R. Roiban, Convergence theorem for noncommutative Feynman graphs and renormalization. JHEP **0103**, 001 (2001). [hep-th/0008090]
8. M. Disertori, V. Rivasseau, Two and three loops beta function of non commutative ϕ_4^4 theory. Eur. Phys. J. C **50**, 661–671 (2007). [hep-th/0610224]
9. M. Disertori, R. Gurau, J. Magnen, V. Rivasseau, Vanishing of beta function of non commutative ϕ_4^4 theory to all orders. Phys. Lett. B **649**, 95–102 (2007). [hep-th/0612251]
10. M.R. Douglas, S.H. Shenker, Strings in less than one dimension. Nucl. Phys. B **335**, 635–654 (1990)
11. V. Gayral, R. Wulkenhaar, Spectral geometry of the Moyal plane with harmonic propagation. J. Noncommut. Geom. **7**, 939–979 (2013). [arXiv:1108.2184 [math.OA]]
12. J.M. Gracia-Bondía, J.C. Várilly, Algebras of distributions suitable for phase space quantum mechanics. I. J. Math. Phys. **29**, 869–879 (1988)
13. D.J. Gross, A.A. Migdal, Nonperturbative two-dimensional quantum gravity. Phys. Rev. Lett. **64**, 127–130 (1990)
14. H. Grosse, R. Wulkenhaar, The β-function in duality-covariant noncommutative ϕ^4-theory. Eur. Phys. J. C **35**, 277–282 (2004). [hep-th/0402093]
15. H. Grosse, R. Wulkenhaar, Power-counting theorem for non-local matrix models and renormalisation. Commun. Math. Phys. **254**, 91–127 (2005). [hep-th/0305066]

16. H. Grosse, R. Wulkenhaar, Renormalisation of ϕ^4-theory on noncommutative $\mathbb{R}^4$ in the matrix base. Commun. Math. Phys. **256**, 305–374 (2005). [hep-th/0401128]
17. H. Grosse, R. Wulkenhaar, Renormalization of ϕ^4-theory on noncommutative $\mathbb{R}^4$ to all orders. Lett. Math. Phys. **71**, 13–26 (2005). [hep-th/0403232]
18. H. Grosse, R. Wulkenhaar, Self-dual noncommutative ϕ^4-theory in four dimensions is a non-perturbatively solvable and non-trivial quantum field theory. Commun. Math. Phys. **329**, 1069–1130 (2014). [arXiv:1205.0465 [math-ph]]
19. H. Grosse, R. Wulkenhaar, Progress in solving a noncommutative quantum field theory in four dimensions. arXiv:0909.1389 [hep-th]
20. H. Grosse, R. Wulkenhaar, Solvable limits of a 4D noncommutative QFT. arXiv:1306.2816 [math-ph]
21. H. Grosse, R. Wulkenhaar, Solvable 4D noncommutative QFT: phase transitions and quest for reflection positivity. arXiv:1406.7755 [hep-th]
22. R. Gurau, V. Rivasseau, Parametric representation of noncommutative field theory. Commun. Math. Phys. **272**, 811 (2007). [math-ph/0606030]
23. R. Gurau, J. Magnen, V. Rivasseau, F. Vignes-Tourneret, Renormalization of non-commutative ϕ^4_4 field theory in x space. Commun. Math. Phys. **267**, 515–542 (2006). [hep-th/0512271]
24. K. Hepp, Proof of the Bogolyubov-Parasiuk theorem on renormalization. Commun. Math. Phys. **2**, 301 (1966)
25. G. Källén, On the definition of the renormalization constants in quantum electrodynamics. Helv. Phys. Acta **25**, 417–434 (1952)
26. T. Krajewski, R. Wulkenhaar, Perturbative quantum gauge fields on the noncommutative torus. Int. J. Mod. Phys. A **15**, 1011–1029 (2000). [hep-th/9903187]
27. P.P. Kulish, Factorization of the classical and quantum S matrix and conservation laws. Theor. Math. Phys. **26**, 132 (1976). [Teor. Mat. Fiz. **26**, 198 (1976)]
28. E. Langmann, R.J. Szabo, Duality in scalar field theory on noncommutative phase spaces. Phys. Lett. B **533**, 168–177 (2002). [hep-th/0202039]
29. H. Lehmann, Über Eigenschaften von Ausbreitungsfunktionen und Renormierungskonstanten quantisierter Felder. Nuovo Cim. **11**, 342–357 (1954)
30. C.P. Martin, D. Sanchez-Ruiz, The one loop UV divergent structure of U(1) Yang-Mills theory on noncommutative $\mathbb{R}^4$. Phys. Rev. Lett. **83**, 476 (1999). [hep-th/9903077]
31. S. Minwalla, M. van Raamsdonk, N. Seiberg, Noncommutative perturbative dynamics. JHEP **0002**, 020 (2000). [hep-th/9912072]
32. J. Moser, Three integrable Hamiltonian systems connected with isospectral deformations. Adv. Math. **16**, 197 (1975)
33. K. Osterwalder, R. Schrader, Axioms for Euclidean Green's functions. Commun. Math. Phys. **31**, 83–112 (1973)
34. K. Osterwalder, R. Schrader, Axioms for Euclidean Green's functions II. Commun. Math. Phys. **42**, 281–305 (1975)
35. J. Polchinski, Renormalization and effective lagrangians. Nucl. Phys. B **231**, (1984) 269.
36. V. Rivasseau, *From Perturbative to Constructive Renormalization* (Princeton University Press, Princeton, 1991)
37. V. Rivasseau, Non-commutative renormalization, in *Quantum Spaces (Séminaire Poincaré X)*, ed. by B. Duplantier, V. Rivasseau (Birkhäuser, Basel, 2007), pp. 19–109. [arXiv:0705.0705 [hep-th]]
38. V. Rivasseau, F. Vignes-Tourneret, R. Wulkenhaar, Renormalisation of noncommutative ϕ^4-theory by multi-scale analysis. Commun. Math. Phys. **262**, 565–594 (2006). [hep-th/0501036]
39. J. Schwinger, Euclidean quantum electrodynamics. Phys. Rev. **115**, 721–731 (1959)
40. R.F. Streater, A.S. Wightman, *PCT, Spin and Statistics, and All That* (Benjamin, New York, 1964)
41. F.G. Tricomi, *Integral Equations* (Interscience, New York, 1957)
42. J.C. Várilly, J.M. Gracia-Bondía, Algebras of distributions suitable for phase-space quantum mechanics. 2. Topologies on the Moyal algebra. J. Math. Phys. **29**, 880–887 (1988)

43. F. Vignes-Tourneret, Renormalization of the orientable non-commutative Gross-Neveu model. Ann Henri Poincare **8**, 427 (2007). [math-ph/0606069]
44. D.V. Widder, The Stieltjes transform. Trans. Am. Math. Soc. **43**, 7–60 (1938)
45. A.S. Wightman, Quantum field theory in terms of vacuum expectation values. Phys. Rev. **101**, 860–866 (1956)
46. K.G. Wilson, Confinement of quarks. Phys. Rev. D **10**, 2445–2459 (1974).
47. W. Zimmermann, Convergence of Bogolyubov's method of renormalization in momentum space. Commun. Math. Phys. **15**, 208 (1969). [Lect. Notes Phys. **558**, 217 (2000)]

Wave Equations with Non-commutative Space and Time

Rainer Verch

Contents

Abstract The behaviour of solutions to the partial differential equation $(D + \lambda W)f_\lambda = 0$ is discussed, where D is a normal hyperbolic partial differential operator, or pre-normal hyperbolic operator, on n-dimensional Minkowski spacetime. The potential term W is a C_0^∞ kernel operator which, in general, will be non-local in time, and λ is a complex parameter. A result is presented which states that there are unique advanced and retarded Green's operators for this partial differential equation if $|\lambda|$ is small enough (and also for a larger set of λ values). Moreover, a scattering operator can be defined if the λ values admit advanced and retarded Green operators. In general, however, the Cauchy-problem will be ill-posed, and examples will be given to that effect. It will also be explained that potential terms arising from non-commutative products on function spaces can be approximated by C_0^∞ kernel operators and that, thereby, scattering by a non-commutative potential can be investigated, also when the solution spaces are (2nd) quantized. Furthermore, a discussion will be given in which the scattering transformations arising from non-commutative potentials will be linked to observables of quantum fields on non-commutative spacetimes through "Bogoliubov's formula". In particular, this helps to shed light on the question how observables arise for quantum fields on Lorentzian spectral geometries.

R. Verch (✉)
Institut für Theoretische Physik, Universität Leipzig, D-04009 Leipzig, Germany
e-mail: rainer.verch@uni-leipzig.de

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_9

Keywords Hyperbolic partial differential operators • Noncommutative spacetime • Quantum field theory

Mathematics Subject Classification (2010). 35L10, 35P25, 81R60, 81T75

1 Introduction

The present contribution essentially reports on the results of a recent article by Gandalf Lechner and the present author [14] to which—often without explicit mentioning—the reader is referred for considerable further details and discussion. The investigation of the said article is embedded in the quest for understanding the relevant structures of quantum field theories on non-commutative spacetimes. There are various ways of approaching this theme, and sometimes the various strands don't seem to connect very well. An approach advocated by the present author [2, 16, 20] is to attempt and combine a general description of non-commutative spacetimes in a framework of Lorentzian spectral geometry [9, 16, 18–20] with the basic principles of local covariant quantum field theory [3, 7]. While this undertaking has some promising aspects from a structural point of view, it is hampered by being very ambitious—perhaps, overly ambitious—from the outset, in that it attempts to design a framework for quantum field theory on a large class of non-commutative spacetimes, despite the fact that it is not even clear if we know what "the general structure" of quantum field theory on a fixed non-commutative spacetime should be. In particular, it is unclear if "the" is an appropriate prefix, as there could be many structurally quite different concepts of quantum field theory on a given non-commutative spacetime which nevertheless appear reasonable for the—hypothetical—physical situation for which they are conceived. Naturally, the idea is to bring a suitably generalized principle of local covariance into play so as to narrow down the potentially vast variety of choices one could make. Judging from the present status of the development of quantum field theory on non-commutative spacetimes, there seems to lie still a long way ahead of us before this could be achieved.

Yet, we will sketch elements of our preferred approach here. The starting point is to set down some rudimentary conditions for a Lorentzian spectral triple, a sort of nucleus for Lorentzian spectral geometry, and to notice that, irrespective of several details (mostly pertaining to the analytical structure of a Lorentzian spectral triple), one can associate a C^*-algebra of canonical anti-commutation relations to any Lorentzian spectral triple. This amounts to an abstract construction of the quantized Dirac field on the—potentially non-commutative—spacetime geometry described by the Lorentzian spectral triple. The usual Minkowski spacetime as well as Moyal deformed Minkowski spacetime will serve as examples. In both examples, one obtains the identical C^* algebra of the quantized Dirac field, and thus there arises the question of how to obtain the information that in the first case one should regard

the C^* algebra as describing the quantized Dirac field on Minkowski spacetime, while in the second case as describing the quantized Dirac field on Moyal deformed Minkowski spacetime. As we will discuss to some extent in Sect. 2, this can be achieved by looking at the action of the algebra $\mathcal{A}$ of the Lorentzian spectral triple on the quantum field operators in the respective cases. This, in turn, may be derived from scattering operators which relate solutions f_λ to the Dirac equation with an "external interaction potential",

$$(D + \lambda V_a) f_\lambda = 0$$

to solutions f_0 of the "free" Dirac equation $Df_0 = 0$, at asymptotically early or late times, akin to potential scattering in quantum mechanics. Here, D is the Dirac operator on Minkowski spacetime, and V_a is an action of an element a of $\mathcal{A}$ on the f_λ which are viewed as elements of the Lorentzian spectral triple's Hilbert space, $\mathcal{H}$.[1] Thus, in the case of Minkowski spacetime, a will typically be a (real-valued) Schwartz function on $\mathbb{R}^4$ and V_a will then amount to pointwise multiplication of f_λ by a, $(V_a f_\lambda)(x) = a(x) f_\lambda(x)$ $(x \in \mathbb{R}^4)$. In contrast, in the case of Moyal deformed Minkowski spacetime, V_a is given by the Moyal product of a and f_λ (see Sect. 2),

$$(V_a f_\lambda)(x) = (a \star f_\lambda)(x) \qquad (x \in \mathbb{R}^4)\,.$$

As will be explained in Sect. 2, the scattering operators obtained from the potential scattering in both situations lead to Bogoliubov transformations α_λ on the C^* algebra of the quantized Dirac field for any a, and differentiation with respect to the coupling strength parameter λ induces operators $X(a)$ (in the Hilbert space of the vacuum representation of the "free" quantized, massless Dirac field on Minkowski spacetime) such that

$$\left.\frac{d}{d\lambda}\right|_\lambda \alpha_\lambda(\Psi(h)) = i[X(a), \Psi(h)]\,.$$

Here, $\Psi(h)$ is a quantized Dirac field operator, and following the line of thought of "Bogoliubov's formula", it may be regarded as an observable of the quantized Dirac field—in this case, linearly dependent on elements a in the algebra $\mathcal{A}$ of the underlying Lorentzian spectral triple. It is the assignment $a \mapsto X(a)$ and the algebraic relations of the $X(a)$ for various a which encode the information that the quantized Dirac field propagates in one case on usual Minkowski spacetime, or in the other case, on Moyal deformed Minkowski spacetime. This conceptual framework can in principle be transferred to more general Lorentzian spectral triples.

[1] ... or as elements of a related, extended space.

At any rate, in order to obtain the assignment $a \mapsto X(a)$, the first step is to obtain scattering operators for a Dirac equation of the form

$$Df_\lambda + \lambda a \star f_\lambda = 0\,.$$

The problem here is that the Moyal product acts non-locally, also with respect to any time-direction on Minkowski spacetime, and therefore one cannot put this equation into the form of a first-order system. However, the operators $V_a f_\lambda = a \star f_\lambda$ can be approximated by operators

$$Wh(x) = \int w(x,y)h(y)d^4y \tag{1}$$

where w is a C_0^∞ kernel (matrix-valued, since h has several components). In [14], we have investigated question of existence and uniqueness of solutions f_λ to the equation

$$(D + \lambda W)f_\lambda = 0 \tag{2}$$

where D is either a 2nd order normal hyperbolic partial differential operator, or a pre-hyperbolic partial differential operator (meaning that D is first order, and there is another first order operator such that DD' and $D'D$ are normal hyperbolic—the Dirac operator is an example) on n-dimensional Minkowski spacetime, and where W is given by a C_0^∞ kernel as in (1). The results of [14], which will be summarized in more detail in Sect. 3, are as follows: If $|\lambda|$ is sufficiently small, then there are unique advanced and retarded fundamental solutions (Green operators) for (2) (and in fact, the Green operators are meromorphic in λ); in general, the Cauchy-problem for (2) is ill-posed (admitting arbitrary W); nevertheless, scattering operators for (2) can be uniquely constructed. We elaborate a bit more on the perspectives of these results for obtaining the operators $X(a)$ mentioned above in the final Sect. 4.

2 Quantum Fields on Lorentzian Spectral Triples

In the spectral geometry approach to non-commutative spaces, the description of a commutative or non-commutative manifold is given in terms of a *spectral triple* $(\mathcal{A}, D, \mathcal{H})$, where $\mathcal{H}$ is a Hilbert space, $\mathcal{A}$ is a $*$-algebra of operators acting in $\mathcal{H}$, and D is a distinguished (unbounded) operator on a suitable domain in $\mathcal{H}$. In the case where the spectral triple corresponds to a "commutative" compact Riemannian manifold with spin structure, $\mathcal{H}$ is formed by the space of L^2 spinor fields on the manifold, $\mathcal{A}$ is the—commutative—$*$-algebra of complex valued functions on the manifold, and D is the Dirac operator. On the other hand, Connes' reconstruction theorem [6] shows that, if a spectral triple has a commutative algebra $\mathcal{A}$, then it actually arises from a compact Riemannian manifold with spin structure in the

way just indicated. That however needs further data objects for a spectral triple and relations among them and, in particular, relations of the additional data objects with the operator D. We refer to [5, 6, 13] for considerable further discussion. At any rate, replacing the commutative algebra $\mathcal{A}$ by a non-commutative algebra (while preserving relations between the data objects) leads to the concept of a non-commutative compact Riemannian manifold in the spectral geometry approach. For examples, see [13].

A physical spacetime is a four-dimensional Lorentzian spacetime and it is usually taken to be globally hyperbolic, and hence non-compact, to avoid causal pathologies. This means that spacetimes do not fit readily into the spectral geometry approach which, therefore, must be suitably generalized to a form of Lorentzian spectral geometry. While such a generalization of spectral geometry doesn't appear to have reached a final form up to now, there is certain progress in this direction [9–11, 16, 18, 19]. The basic idea is that a Lorentzian spectral geometry is again described by a spectral triple $(\mathcal{A}, D, \mathcal{H}, \mathsf{x}_i)$ but with further data objects x_i which are different from the compact Riemannian manifold case mentioned before, and have different relations among each other, and with D. As mentioned, the discussion has not reached a final form as to what the x_i and their relations are. However, for any promising choice, it is expected that the following holds: [4pt] Suppose two (globally hyperbolic) Lorentzian spacetimes $\boldsymbol{M}$ and $\tilde{\boldsymbol{M}}$ (with spin structures) are described by Lorentzian spectral triples $(\mathcal{A}, D, \mathcal{H}, \mathsf{x}_i)$ and $(\tilde{\mathcal{A}}, \tilde{D}, \tilde{\mathcal{H}}, \tilde{\mathsf{x}}_i)$. Then the two Lorentzian spectral triples are unitarily equivalent if and only if $\boldsymbol{M}$ and $\tilde{\boldsymbol{M}}$ are isometric with equivalent spin structures. Here, the two Lorentzian spectral triples are called unitarily equivalent if there is a unitary operator $U : \mathcal{H} \to \tilde{\mathcal{H}}$ such that

$$\tilde{\mathcal{A}} = U\mathcal{A}U^{-1}\,,\quad \tilde{\mathsf{x}}_i = U\mathsf{x}_iU^{-1}\,,\quad [\,[\tilde{D}, UaU^{-1}], \tilde{b}\,] = [U[D, a]U^{-1}, \tilde{b}] \tag{3}$$

for all $a \in \mathcal{A}$, $\tilde{b} \in \tilde{\mathcal{A}}$, where $[A, B] = AB - BA$. [6pt] Let us introduce the abbreviations $\boldsymbol{L} = (\mathcal{A}, D, \mathcal{H}, \mathsf{x}_i)$ for a Lorentzian spectral triple and $\boldsymbol{L} \xrightarrow{\psi_U} \tilde{\boldsymbol{L}}$ for a unitary equivalence morphism between spectral triples induced by a unitary U as in (3).

At this point it is in order to briefly mention the basic structure of local covariant quantum field theory (see [3, 7] for further details not elaborated on in these writings). A local covariant quantum field theory consists of an assignment $\boldsymbol{M} \to \mathscr{A}(\boldsymbol{M})$ of $*$-algebras (or C^*-algebras) to globally hyperbolic spacetimes $\boldsymbol{M}$. The $\mathscr{A}(\boldsymbol{M})$ are the algebras of observables, or more generally, of the quantum field (of a given type) on the spacetime $\boldsymbol{M}$. Additionally, whenever there is an isometric hyperbolic embedding $\boldsymbol{M} \xrightarrow{\psi} \tilde{\boldsymbol{M}}$—i.e. if $\boldsymbol{M}$ can be viewed as a globally hyperbolic sub-spacetime of $\tilde{\boldsymbol{M}}$—then there should be an injective $*$-algebra morphism $\mathscr{A}(\boldsymbol{M}) \xrightarrow{\alpha_\psi} \mathscr{A}(\tilde{\boldsymbol{M}})$; moreover, the composition law $\alpha_{\psi_1\circ\psi_2} = \alpha_{\psi_1} \circ \alpha_{\psi_2}$ is required to hold. Expressed in more mathematical terms, this says that a local covariant quantum field theory is a functor from the category of globally hyperbolic spacetimes (all four-dimensional), with isometric hyperbolic embeddings as arrows,

to the category of $*$-algebras, with monomorphisms as arrows. The interesting point is that this does not amount to just dressing up quantum field theory on general spacetime manifolds in a fancy mathematical coat, but that it has led to significant new insights and results in quantum field theory in curved spacetimes. We will not report on this issue here any further but just refer to the recent survey [8] and literature cited there for a fuller discussion.

It is suggestive to try and carry over this line of approach to quantum field theory on non-commutative spacetimes essentially by replacing the category of globally hyperbolic spacetimes by the category of Lorentzian spectral triples with unitary equivalences as arrows—for a start (this is certainly not general enough; see remark to follow). Then a "covariant" quantum field theory on Lorentzian non-commutative spacetimes should be given by an assignment $\boldsymbol{L} \to \mathscr{A}(\boldsymbol{L})$ of a $*$-algebra $\mathscr{A}(\boldsymbol{L})$ to any Lorentzian spectral triple $\boldsymbol{L}$ together with injective $*$-algebra morphisms $\mathscr{A}(\psi_U)$ for any unitary equivalence $\boldsymbol{L} \stackrel{\psi_U}{\longrightarrow} \tilde{\boldsymbol{L}}$ featuring the functorial property $\mathscr{A}(\psi_{U_1}) \circ \mathscr{A}(\psi_{U_2}) = \mathscr{A}(\psi_{U_1 U_2})$.

The remark that this is not enough is in order now. One of the strengths of the local covariant framework for quantum field theory stems from the fact that an embedding of a spacetime into a larger one is accompanied by an embedding of the corresponding quantum field theories. One would have to devise a similar embedding for Lorentzian spectral triples which gives similarly rise to an embedding of the associated quantum field theory. It is not clear what a suitable concept of embedding of Lorentzian spectral triples, to this end, would amount to. A first working hypothesis might be to replace the unitary U by a partial isometry, or a partial isometry combined with a suitable generalization of the equalities in (3) as holding only up to "negligible corrections", an idea which is in fact of some importance in spectral geometry [5, 13, 16]. At any rate, one encounters the problem of what replaces the concept of locality in quantum field theory on non-commutative spacetimes at this point.

We are hopeful that our investigation reported on here will contribute to gaining further understanding of these matters. To illustrate how we hope to approach that matter, we will be more concrete and consider a very simple model for a non-commutative version of Minkowski spacetime, the Moyal-deformed Minkowski spacetime. As we have mentioned before, it is not entirely clear what the assumptions on a Lorentzian spectral triple ultimately should be, but in case they were set up in such a way that Moyal-deformed Minkowski spacetime does not fit into the framework, then the list of examples of quantum field theories on non-commutative Lorentzian spectral triple spacetimes would run thin indeed. Therefore, we anticipate that Moyal-deformed Minkowski spacetime (as well as Minkowski spacetime as such) can be modelled as Lorentzian spectral triples. To that end, the primary indication and motivation comes from the discussion in [12] (see also [2]) where Moyal planes are described as generalized Riemannian spectral triples. That description can be given a Lorentzian variant which one would expect to bear central features of Lorentzian spectral geometry. We outline it here, very crudely. A Lorentzian spectral triple for "commutative" Minkowski

spacetime would start from taking a Hilbert space, $\mathcal{H}$, of L^2 spinors on Minkowski spacetime. There is no Poincaré covariant notion of L^2 spinors on Minkowski spacetime but there are many possible choices depending on a choice of time direction; consequently, the choice made will be recorded and forms a piece of data of the spectral geometry. The algebra $\mathcal{A}$ can be taken to be $\mathscr{S}(\mathbb{R}^4)$, the Schwartz functions on Minkowski spacetime, with their commutative pointwise multiplication as algebra product. The obvious choice for D is the usual Lorentzian Dirac operator on Minkowski spacetime. To obtain a Lorentzian spectral triple for Moyal-deformed Minkowski spacetime, one only needs to replace the commutative algebra $\mathscr{S}(\mathbb{R}^4)$ by $\mathscr{S}_\star(\mathbb{R}^4)$, the Schwartz functions with the non-commutative Moyal product[2]

$$f \star h = \int_{\mathbb{R}^4} d^4p \int_{\mathbb{R}^4} d^4z \, \mathrm{e}^{2\pi i(p\cdot z)} f(x-\theta p)h(x-z) \tag{4}$$

as algebra product, rendering a non-commutative algebra $\mathcal{A}$. (For more details, see the references [4, 12, 17].)

The next step of interest to us is setting up a quantum field theory on Minkowski spacetime given in form of a Lorentzian spectral triple. Since spinors and the Dirac operator appear in that description of Minkowski spacetime, as a beginning step it appears most natural to start with the free quantized Dirac field. There is indeed a very simple way of associating to the Lorentzian spectral triple $\boldsymbol{L}_0 = (\mathscr{S}(\mathbb{R}^4), D, \mathcal{H})$ of Minkowski space the quantized Dirac field: By defining $\mathscr{F}(\boldsymbol{L}_0)$ as the CAR algebra—algebra of canonical anti-commutation relations—which is the unique C^*-algebra generated by a unit element $\mathbf{1}$ and by elements $\Psi(f)$, $f \in \mathcal{H}$, with the properties:

$$\begin{aligned}
&(1) \quad f \mapsto \Psi(f) \quad \text{is linear}\,,\\
&(2) \quad \Psi(Df) = 0\,,\\
&(3) \quad \Psi(f)^* = \Psi(\Gamma f)\,,\\
&(4) \quad \Psi(f)^*\Psi(h) + \Psi(h)\Psi(f)^* = i\langle f, \gamma_0 R h\rangle \mathbf{1}\,.
\end{aligned}$$

Here, the Γ appearing on the right hand side of (3) is a preferred complex conjugation on $\mathcal{H}$ which is actually contained (previously unmentioned) in the full list of data for a Lorentzian spectral triple. In (4), the notation used is: $\langle f, h\rangle$ is the scalar product of the Hilbert space $\mathcal{H}$, and γ_0 is an operator on $\mathcal{H}$ which is a further datum of the Lorentzian spectral triple carrying the information about the time-direction that has been chosen to obtain a Lorentzian scalar product on the spinors. Incidentally, in the example at hand, γ_0 coincides with the Dirac matrix γ_0 if $\mathcal{H}$ is

[2] where $(p\cdot z) = \sum_{\mu=0,\ldots,3} p_\mu z_\mu$ is the Euclidean scalar product on $\mathbb{R}^4$ and θ is a real invertible symplectic 4×4 matrix which is kept fixed (and usually chosen with $\det(\theta) = 1$).

taken as $L^2(\mathbb{R}^4, \mathbb{C}^4)$ with scalar product

$$\langle f, h\rangle = \sum_{A=0}^{3} \int_{\mathbb{R}^4} \bar{f}_A(x) h_A(x)\, d^4x \tag{5}$$

Finally, $R = R^+ - R^-$ is the difference of retarded and advanced fundamental solutions to the Dirac operator D which are defined as (suitably continuous) linear operators $R^\pm : \mathscr{S}(\mathbb{R}^4, \mathbb{C}^4) \to C^\infty(\mathbb{R}^4, \mathbb{C}^4)$ such that

$$DR^\pm f = R^\pm Df = f \text{ and } \operatorname{supp}(R^\pm f) \subset J^\pm(\operatorname{supp}(f)) \tag{6}$$

where $J^\pm(\operatorname{supp}(f))$ means causal future (+) / causal past (−) of $\operatorname{supp}(f)$ in Minkowski spacetime. In this case, it turns out that $i\langle f, \gamma_0 Rh\rangle$ endows $\mathscr{S}(\mathbb{R}^4)$ with a semi-definite sesquilinear form, and the kernel of that form coincides with the kernel of R.

This defines the algebra $\mathscr{F}(\boldsymbol{L}_0)$ of the Lorentzian spectral triple of Minkowski spacetime and it actually coincides with the usual CAR algebra of the quantized Dirac field in Minkowski spacetime. One observes that $\mathscr{F}(\boldsymbol{L}_0)$ is nothing more than an abstract "2nd quantization" of the Hilbert space $\mathcal{H}$ (together with the complex conjugation Γ) of $\boldsymbol{L}_0$. Moreover, one also readily observes that the algebra $\mathcal{A} = \mathscr{S}(\mathbb{R}^4)$ appearing in $\boldsymbol{L}_0$ does not enter the construction of $\mathscr{F}(\boldsymbol{L}_0)$. On the one hand, that can be taken as an advantage since it allows it to directly generalize the construction of $\mathscr{F}(\boldsymbol{L}_0)$ from $\boldsymbol{L}_0$ to the case of $\boldsymbol{L}_\star = (\mathscr{S}_\star(\mathbb{R}^4), D, \mathcal{H})$. Clearly, this results in $\mathscr{F}(\boldsymbol{L}_\star) = \mathscr{F}(\boldsymbol{L}_0)$ since, as mentioned, the data of $\boldsymbol{L}_0$ and $\boldsymbol{L}_\star$ are identical apart from the different algebras $\mathscr{S}(\mathbb{R}^4)$ and $\mathscr{S}_\star(\mathbb{R}^4)$ which however don't appear in the construction. On the other hand, that invokes the question where the information is stored that $\mathscr{F}(\boldsymbol{L}_\star)$ is the algebra of the quantized Dirac field on the non-commutative Moyal-deformed Minkowski spacetime whereas $\mathscr{F}(\boldsymbol{L}_0)$ is the algebra of the quantized Dirac field on the classical, "commutative" Minkowski spacetime. Obviously, in order to see the difference, one needs some kind of action of the algebras $\mathscr{S}_\star(\mathbb{R}^4)$ and $\mathscr{S}(\mathbb{R}^4)$, respectively, on the algebra of the quantized Dirac field.

One possible such action can be derived from a scattering situation. Let a be a (real) test-function of Schwartz type on $\mathbb{R}^4$. Regarding a as an element of the commutative algebra $\mathscr{S}(\mathbb{R}^4)$, one can modify the free Dirac equation $Df_0 = 0$ to the Dirac equation

$$(D + \lambda V_a) f_\lambda = 0 \tag{7}$$

with a potential term V_a and small (real) parameter λ, where

$$(V_a f)(x) = a(x) f(x) \tag{8}$$

is just the action of the Schwartz function a on a spinor field (to be thought of as an element in $\mathcal{H}$) by pointwise multiplication. On the other hand, if a is interpreted as an element in $\mathscr{S}_\star(\mathbb{R}^4)$, then the potential term V_a takes e.g. the form

$$(V_a f)(x) = a \star f(x)\,. \tag{9}$$

Now one can investigate the scattering problem of the Dirac equation with any of the potentials V_a of (8) or (9). This, as we will see, renders an action of a on the field operators $\Psi(f)$. Let us recall how that proceeds for the potential V_a in the commutative case (8): Here, one can put the field equation (7) in "Hamiltonian form" (or "first order form"). That means, denoting by $u_{\lambda,t}(\mathbf{x}) = f_\lambda(t, \mathbf{x})$ the Cauchy-data at time t of a solution f_λ to (7), f_λ is a solution iff the $u_{\lambda,t}$ satisfy a first-order differential equation of the form

$$\frac{d}{dt}u_{\lambda,t} + A_{\lambda,t}u_{\lambda,t} = 0 \tag{10}$$

where $A_{\lambda,t}$ is, at each t, a partial differential operator acting with respect to the spatial $\mathbf{x}$-coordinates (with t-dependent coefficients). In fact, a large class of partial differential equations can be cast into this form, which often facilitates proving existence and uniqueness of solutions to given Cauchy-data at some given value of time t. Then one can define propagation operators $T_{\lambda,t} : u_{\lambda,0} \mapsto u_{\lambda,t}$ mapping data of a solution at time 0 to the data at time t. Consequently, one can study the scattering problem in complete analogy to the scattering problem in quantum mechanics, in first defining the Møller operators

$$\Omega_{\lambda,\pm} = \lim_{t\to\pm\infty} T_{0,t}(T_{\lambda,t})^{-1} \tag{11}$$

and consequently, the scattering operator (here still at "one-particle level"),

$$\boldsymbol{s}_\lambda = \Omega_{\lambda,+}(\Omega_{\lambda,-})^{-1}\,. \tag{12}$$

Under very general conditions, that scattering operator—mapping a solution f_0 of the Dirac equation $Df_0 = 0$ to another solution $\boldsymbol{s}_\lambda f_0$, i.e. $D\boldsymbol{s}_\lambda f_0 = 0$—induces a C^*-algebra morphism α_λ on the algebra $\mathscr{F}(\boldsymbol{L}_0)$ of the quantized Dirac field on Minkowski spacetime by

$$\alpha_\lambda(\Phi(f_0)) = \Phi(\boldsymbol{s}_\lambda f_0) \tag{13}$$

with

$$\Phi(Rh) = \Psi(h) \tag{14}$$

i.e. the $\Phi(f_0)$ are again algebraic generators of the CAR-algebra of the quantized Dirac field, but labelled by solutions f_0 to the "free" Dirac equation $Df_0 = 0$,

whereas the $\Psi(h)$ are labelled by test-functions; the connection between these operators is a consequence of $\Psi(Dh) = 0$.

Then one can differentiate $\alpha_\lambda(\Phi(f_0))$ with respect to the coupling strength parameter λ, evaluated at $\lambda = 0$,

$$\boldsymbol{\delta}_a(\Phi(f_0)) = \frac{d}{d\lambda}\bigg|_{\lambda=0} \alpha_\lambda(\Phi(f_0)) = \Phi(\boldsymbol{d}_a f_0) \tag{15}$$

where

$$\boldsymbol{d}_a f_0 = RV_a f_0\,, \tag{16}$$

i.e. pointwise multiplication of the solution f_0 to the free Dirac equation by a followed by application of the advanced-minus-retarded Green operator R to produce again a solution to the free Dirac equation. One can check that

$$\boldsymbol{\delta}_a(\Phi(f_0)) = i[:\Psi^+\Psi:(a), \Phi(f_0)] \tag{17}$$

where $:\Psi^+\Psi:$ is the normal-ordered squared Dirac field operator. (Here interpreted in the vacuum representation of the "free", i.e. massless Dirac field; Ψ^+ is the Dirac-adjoint field to Ψ.) Thus, (17) can be seen as an instance of "Bogoliubov's formula", deriving observable fields from differentiating an S-matrix, or the corresponding scattering transformation (in our case, α_λ) with respect to the interaction strength.

This provides already a hint on how one can expect the algebra $\mathcal{A}$ to make an appearance when setting up a quantum field theory over a Lorentzian spectral triple: In the present case, that would occur via the operators $:\Psi^+\Psi:(a)$ which are to be regarded as observables of the quantized Dirac field (they correspond to the "squared field strength" weighted with a as smearing function).

Now we would like to implement a similar line of thought in the case of the quantized Dirac field on Moyal deformed Minkowski spacetime and find counterparts to the $:\Psi^+\Psi:(a)$ in this case, which then provides a handle on how $\mathscr{S}_\star(\mathbb{R}^4)$ comes in play with the algebra $\mathscr{F}(\boldsymbol{L}_\star)$—and how this interplay differs from the case of classical Minkowski spacetime. At that point, one encounters a difficulty: The potential term V_a of (9) is highly non-local, in particular, it is non-local in time. This circumstance prevents turning the Dirac equation (7) into a first-order system of the form (10). Nevertheless, as will be mentioned in Sect. 4, it is still possible to obtain (approximate) Møller operators and scattering operators for solutions to (7), and thereby, implement "Bogoliubov's formula" also for the quantized Dirac field on Moyal deformed Minkowski spacetime. We should like to point out that this approach of gaining observables of the quantized Dirac field over some Lorentzian spectral triple is applicable generally—i.e. in principle beyond Moyal-like deformations of Minkowski spacetime—once one can define the scattering morphisms α_λ or their derivations $\boldsymbol{\delta}_a$ for the requisite V_a corresponding to the Lorentzian spectral triple at hand. In fact, as we will point out later, it works in similar fashion for the localized Moyal-like deformations of Minkowski spacetime

considered by Waldmann et al. [1, 15] although these non-commutative geometries have, at present, not been described in terms of Lorentzian spectral triples.

3 Wave Equations with Non-local C_0^∞ Kernel Operators as Potential Terms

In this section we will summarize the results of [14] on the solution behaviour of partial differential equations of the form

$$D_\lambda f_\lambda = (D + \lambda W) f_\lambda = 0 \tag{18}$$

where D is a normal hyperbolic operator, or pre-normal hyperbolic operator, and f_λ is in $C^\infty(\mathbb{R}^n, \mathbb{C}^N)$, W is a C_0^∞-kernel operator, and λ is a complex parameter. The requisite definitions from [14] are as follows:

Definition 3.1

1. A linear differential operator D on $C^\infty(\mathbb{R}^n, \mathbb{C}^N)$ is called *normally hyperbolic* if there exist smooth matrix-valued functions $U^0, \ldots, U^s, V : \mathbb{R}^n \to \mathbb{C}^{N\times N}$ such that

$$D = \frac{\partial^2}{\partial x_0^2} - \sum_{k=1}^{s} \frac{\partial^2}{\partial x_k^2} + \sum_{\mu=0}^{s} U^\mu(x) \frac{\partial}{\partial x_\mu} + V(x)\,. \tag{19}$$

2. A linear differential operator D on $C^\infty(\mathbb{R}^n, \mathbb{C}^N)$ is called *pre-normally hyperbolic* if D is of first order, and there exists another first order differential operator D' on $C^\infty(\mathbb{R}^n, \mathbb{C}^N)$ such that $D'D$ and DD' are normally hyperbolic.
3. A C_0^∞-kernel operator is a mapping $W : C^\infty(\mathbb{R}^n, \mathbb{C}^N) \to C^\infty(\mathbb{R}^n, \mathbb{C}^N)$ which can be represented as

$$(Wf)(x) := \int dy\, w(x, y) f(y)\,, \qquad f \in C^\infty(\mathbb{R}^n, \mathbb{C}^N), \tag{20}$$

where $w \in C_0^\infty(\mathbb{R}^n \times \mathbb{R}^n, \mathbb{C}^{N\times N})$. The family of all C_0^∞-kernel operators will be denoted by $\mathcal{W}$.

As was already mentioned in the previous section, a normal hyperbolic or pre-normal hyperbolic operator D possesses unique advanced and retarded fundamental solutions (or Green operators) $R^\pm : C_0^\infty(\mathbb{R}^n, \mathbb{C}^N) \to C^\infty(\mathbb{R}^n, \mathbb{C}^N)$ which are characterized by the properties (6). The main result of [14], summarized in the subsequent Theorem 3.2, states that this holds also for $D_\lambda = D + \lambda W$ where D is (pre-) normal hyperbolic and $W \in \mathcal{W}$ provided that $|\lambda|$ is small enough, and even more generally. However, owing to the non-local action of W in general, the support properties of the Green-operators will not reflect the causal propagation behaviour as in (6). (For a graphical illustration, see [14].)

Theorem 3.2 *Let $D_\lambda = D + \lambda W$ where D is a normal hyperbolic or pre-normal hyperbolic operator on $C^\infty(\mathbb{R}^n, \mathbb{C}^N)$, and $W \in \mathcal{W}$, $\lambda \in \mathbb{C}$. Suppose that* $\mathrm{supp}(w) \subset K \times K$ *for some compact subset K of $\mathbb{R}^n$ where w is the kernel function of W. $R^\pm$ are the advanced/retarded Green operators of D.*

For sufficiently small $|\lambda|$, there are unique continuous linear operators $R^\pm_\lambda : C^\infty_0(\mathbb{R}^n, \mathbb{C}^N) \to C^\infty(\mathbb{R}^n, \mathbb{C}^N)$ such that for any $f, g \in C^\infty_0(\mathbb{R}^n, \mathbb{C}^N)$, the following relations hold[3]*:*

1. $D_\lambda R^\pm_\lambda f = f = R^\pm_\lambda D_\lambda f$.
2. $\mathrm{supp}(R^\pm_\lambda f) \subset J^\pm(\mathrm{supp} f) \cup J^\pm(K)$.
3. $\mathrm{supp}(R^\pm_\lambda f - R^\pm f) \subset J^\pm(K)$.
4. *If* $J^\pm(\mathrm{supp} f) \cap K = \emptyset$, *then* $R^\pm_\lambda f = R^\pm f$.
5. *If D and W are symmetric, i.e. $D = D^*$, $W = W^*$, and $\lambda \in \mathbb{R}$, then one has, for any $f, g \in C^\infty_0(\mathbb{R}^n, \mathbb{C}^N)$,*

$$\langle g, R^\pm_\lambda f\rangle = \langle R^\mp_\lambda g, f\rangle\,, \tag{21}$$

where the scalar product $\langle\,.\,,\,.\,\rangle$ is defined analogously as in (5). Moreover, the dependence of $R^\pm_\lambda$ on λ is meromorphic (in a suitable topology)[4] *so that operators $R^\pm_\lambda$ with the stated properties exist for all λ values except for a nowhere dense set.*

For the proof, we refer to [14].

As mentioned already, since W will in general act non-locally (in space and time), one cannot expect that the partial differential equation (18) admits a well-posed Cauchy problem, even if λ is chosen such that the unique advanced and retarded Green operators $R^\pm_\lambda$ exist. We present two examples from [14] illustrating such behaviour. The first example shows that one may construct a W together with C^∞_0 initial data on a Cauchy surface such that there is no solution f_λ to (18) with the prescribed Cauchy data and $\lambda \neq 0$.

Proposition 3.3 *Let $D = \Box$ be the d'Alembert operator, Σ a Cauchy hyperplane, and $Wh := \langle w_1, h\rangle w_2$ with $w_1, w_2 \neq 0$ C^∞_0 functions on $\mathbb{R}^n$ such that* $\mathrm{supp}\, w_1 \subset \mathcal{O}_1$, $\mathrm{supp}\, w_2 \subset \mathcal{O}_2$ *with two spacelike separated double cones $\mathcal{O}_1$, $\mathcal{O}_2$ based on Σ.*[5] *Pick Cauchy data u on Σ supported in $\mathcal{O}_1$ such that $f_0[u]$, the unique solution to $Df_0[u] = 0$ with these Cauchy data, satisfies $\langle w_1, f_0[u]\rangle \neq 0$, and also assume that $Rw_2 \neq 0$. Then there exists no solution f_λ to (18) with $\lambda \neq 0$ and Cauchy data u.*

[3] In the present context, $\mathbb{R}^n$ is viewed as n-dimensional Minkowski spacetime with metric $(+, -, \ldots, -)$, and time-direction corresponding to increasing x^0-coordinate; $J^\pm(G)$ are the causal future/past sets of $G \subset \mathbb{R}^n$.

[4] Thanks are due to Alexander Strohmaier for pointing this out.

[5] That means that $\mathcal{O}_j = \mathrm{D}(\Sigma_j)$ where Σ_j are open subsets of Σ and $\mathrm{D}(\Sigma_j)$ denotes the open domain of dependence.

The next example from [14] shows that solutions to (18) are in general not uniquely determined by Cauchy-data.

Proposition 3.4 *Let $D = \Box$ be the d'Alembert operator, $Wf = \langle w_1, f\rangle w_2$, with w_1, w_2 C_0^∞ functions on $\mathbb{R}^n$ having spacelike separated supports, and let Σ be a Cauchy hyperplane such that* $\operatorname{supp} w_2 \subset \Sigma^-$*, where Σ^- denotes the open causal past of Σ (excluding Σ). Denoting the Cauchy data of Rw_2 on Σ by u, let $f_\lambda := f_0[u] - R^+ w_2$. Then w_1 and $\lambda \neq 0$ can be chosen in such a way that the $R_\lambda^\pm$ exist, f_λ is a non-zero solution to $D_\lambda f_\lambda = 0$, and f_λ has zero Cauchy data on Σ.*

For proofs of these propositions and graphical illustrations of the situations, we refer again to [14].

Despite these difficulties, one can still show that there are uniquely determined Møller operators as well as scattering operators as soon as the Green operators $R_\lambda^\pm$ exist. To describe the result obtained to this end in [14], we need to collect some notation. Given D and W as before, we write $R_\lambda = R_\lambda^+ - R_\lambda^-$ and $\mathrm{Sol}_\lambda = R_\lambda C_0^\infty(\mathbb{R}^n, \mathbb{C}^N)$ for the space of solutions f_λ to (18) obtained from the Green operators (always assuming $|\lambda|$ sufficiently small so that $R_\lambda^\pm$ exist uniquely). We usually write $R = R_0$, in keeping with previously used notation. Again we assume that $\mathrm{supp}(w) \subset K \times K$ where K is some compact subset of $\mathbb{R}^n$, and we select two Cauchy-surfaces, $\Sigma_{\tau_\pm}$, such that K is in the timelike past of Σ_{τ_+} and in the timelike future of Σ_{τ_-}. With these conventions, we can define the Møller operators

$$\Omega_{\lambda,\pm} : \mathrm{Sol}_\lambda \to \mathrm{Sol}_0\,, \quad \Omega_{\lambda,\pm}(R_\lambda h) = Rh \quad (h \in C_0^\infty(\Sigma_{\tau_\pm}^\pm, \mathbb{C}^N)) \tag{22}$$

where $\Sigma_{\tau_+}^+$ is the open causal future of Σ_{τ_+} and $\Sigma_{\tau_-}^-$ is the open causal past of Σ_{τ_-}. Therefore, $\Omega_{\lambda,-}$ assigns to a solution $f_\lambda = R_\lambda h$ to the "interacting" equation of motion $D_\lambda f_\lambda = 0$ the solution $f_0 = Rh$ to the "free" equation of motion $Df_0 = 0$ which coincides with f_λ everywhere sufficiently in the past of the interaction region K. This assignment is unambiguous in view of Theorem 3.2, Item 4. The action of $\Omega_{\lambda,+}$ is analogous, interchanging the past of the interaction region K with its future. Consequently, one can define the scattering operator

$$\boldsymbol{s}_\lambda : \mathrm{Sol}_0 \to \mathrm{Sol}_0\,, \quad \boldsymbol{s}_\lambda = \Omega_{\lambda,+}(\Omega_{\lambda,-})^{-1}\,. \tag{23}$$

The following statement lists parts of the results in [14].

Theorem 3.5

(*a*) *The Møller operators $\Omega_{\lambda,\pm}$ and the scattering operator $\boldsymbol{s}_\lambda$ are linear bijections.*
(*b*) *The scattering operator can be represented as*

$$\boldsymbol{s}_\lambda = 1 + RW \sum_{k=0}^{\infty} \lambda^{k+1} (-R^+ W)^k$$

and the series converges in the operator norm on $L^2([-\tau,\tau]\times\mathbb{R}^{n-1},\mathbb{C}^N)$ *where* $[-\tau,\tau]$ *is a finite but sufficiently large time interval.*

(*c*) *For any* $f_0 \in \mathrm{Sol}_0$,

$$\lambda \mapsto \boldsymbol{s}_\lambda f_0 \tag{24}$$

is analytic in the nuclear topology of $C_0^\infty(\mathbb{R}^n,\mathbb{C}^N)$ *on a finite disc around* $\lambda = 0$. *In particular, given* $f_0 \in \mathrm{Sol}_0$, *then*

$$\left.\frac{d(\boldsymbol{s}_\lambda f_0)}{d\lambda}\right|_{\lambda=0} = RWf_0\,. \tag{25}$$

4 Discussion and Perspective

One can show that the scattering operator $\boldsymbol{s}_\lambda$ induces, for sufficiently small (real) λ a Bogoliubov transformation on the CAR algebra (if D is Dirac operator) which provides an abstract 2nd quantization of the Dirac field (i.e. of the solution space Sol_0), as we have sketched in Sect. 2. Similarly, $\boldsymbol{s}_\lambda$ induces a Bogoliubov transformation on the CCR algebra which describes an abstract 2nd quantization of a Bosonic field in the case that D is a hyperbolic (wave-type) operator. Moreover, one can establish the relations (15) and (16) for both the CAR and CCR quantized cases. For details, see [14].

There is also the following generalization: Suppose that there is an operator W on $C^\infty(\mathbb{R}^n,\mathbb{C}^N)$ which is no C_0^∞ kernel operator, but such that there is a sequence W_ν, $\nu\in\mathbb{N}$, of C_0^∞ kernel operators which approximate W "suitably". That means, in particular, that (for the CAR/quantized Dirac field case) the derivations

$$\boldsymbol{\delta}_{(\nu)}(\Phi(f_0)) = \left.\frac{d}{d\lambda}\right|_{\lambda=0} \alpha_{W_\nu,\lambda}(\Phi(f_0)) = \Phi(RW_\nu f_0)\,, \tag{26}$$

which are obtained from the scattering operators $\boldsymbol{s}_{W_\nu,\lambda}$ corresponding to the potential terms W_ν, should converge in the limit $\nu\to\infty$ to a derivation on the algebra of field operators of the quantized Dirac field (in vacuum representation). That is in fact expected to hold when taking $Wh = a\star h$ for a Schwartz function a and the Moyal product (4) with invertible θ; it has been proved to hold in the case that θ is degenerate and has no non-zero "time-time" components [2]. It is likewise expected to hold when taking $Wh = a\circledast h$ where $\circledast$ denotes a local non-commutative product introduced by Stephan Waldmann and co-authors [1, 15]; see again [14] for further discussion on this point. In fact, this should be obtainable by standard arguments, and we hope to return to this issue elsewhere. Assuming that convergence of $\boldsymbol{\delta}_{(\nu)}$ to a derivation $\boldsymbol{\delta}_W \equiv \boldsymbol{\delta}_a$ can be established in the mentioned cases, one anticipates, as discussed in Sect. 2, that there is an assignment $a\mapsto X(a)$ of elements a in the "non-commutative spacetime algebra" to quantum field operators $X(a)$ that renders

$\delta_a(\Psi(h)) = i[X(a), \Psi(h)]$. The non-commutativity of the elements of the spacetime algebra is then reflected in algebraic relations of the $X(a)$ for different a, e.g. in the behaviour of the commutator $[X(a_1), X(a_2)]$. However, depending on the non-commutative structure of the algebra $\mathcal{A}$ from which the a_j are taken, it is likely that useful properties of $[X(a_1), X(a_2)]$ could only be derived for special elements a_1, a_2 of $\mathcal{A}$. For instance, in case of $\mathcal{A} = \mathscr{S}_\star(\mathbb{R}^4)$, the elements of the oscillator basis of the Moyal plane are promising candidates. This should furthermore shed a light on potentially useful generalized locality concepts for quantum field theories on non-commutative spacetimes, within the Lorentzian spectral triple approach as well as beyond.

Acknowledgements Thanks are due to Alexander Strohmaier as indicated in a footnote in Sect. 2. Thanks are also extended to the participants of the conference "Quantum Mathematical Physics", Regensburg, 2014, for remarks and comments. I would also like to thank the organizers and sponsoring institutions of that conference for financial support.

References

1. D. Bahns, S. Waldmann, Locally noncommutative spacetimes. Rev. Math. Phys. **19**, 272–306 (2007)
2. M. Borris, R. Verch, Dirac field on Moyal-Minkowski spacetime and non-commutative potential scattering. Commun. Math. Phys. **293**, 399–448 (2010)
3. R. Brunetti, K. Fredenhagen, R. Verch, The generally covariant locality principle – a new paradigm for local quantum physics. Commun. Math. Phys. **237**, 31 (2003)
4. D. Buchholz, G. Lechner, S.J. Summers, Warped convolutions, Rieffel deformations and the construction of quantum field theories. Commun. Math. Phys. **304**, 95–123 (2011)
5. A. Connes, *Noncommutative Geometry* (Academic Press, San Diego, 1994)
6. A. Connes, On the spectral characterization of manifolds. J. Noncommutative Geom. **7**, 1–82 (2013)
7. C.J. Fewster, R. Verch, Dynamical locality and covariance: what makes a physical theory the same in all spacetimes? Ann. Henri Poincaré **13**, 1613–1674 (2012)
8. C.J. Fewster, R. Verch, *Algebraic Quantum Field Theory in Curved Spacetimes* (2015, forthcoming)
9. N. Franco, Lorentzian approach to non-commutative geometry. Ph.D. thesis, Univ. Notre Dame de la Paix, Namur, 2011. arXiv:1108:0592[math-ph]
10. N. Franco, M. Eckstein, An algebraic formulation of causality for noncommutative geometry. Class. Quantum Gravity **30**, 135007 (2013)
11. N. Franco, M. Eckstein, Noncommutative geometry, Lorentzian structures and causality. arXiv:1409.1480[math-ph]
12. V. Gayral, J.M. Gracia-Bondia, B. Iochum, T. Schucker, J.C. Varilly, Moyal planes are spectral triples. Commun. Math. Phys. **246**, 569–623 (2004)
13. J.M. Gracia-Bondia, J.C. Várilly, H. Figueroa, *Elements of Noncommutative Geometry*. Birkhäuser Advanced Texts (Birkhäuser, Boston/Basel/Berlin, 2001)
14. G. Lechner, R. Verch, Linear hyperbolic PDEs with non-commutative time. J. Noncommutative Geom. (to appear). arXiv:1307.1780[math-ph]
15. G. Lechner, S. Waldmann, Strict deformation quantization of locally convex algebras and modules. arXiv:1109.5950[math-ph]

16. M. Paschke, R. Verch, Local covariant quantum field theory over spectral geometries. Class. Quantum Gravity **21**, 5299 (2004)
17. M.A. Rieffel, *Deformation Quantization for Actions of* R^d. Memoirs of the American Mathematical Society, vol. 106 (American Mathematical Society, Providence, 1992)
18. A. Strohmaier, On noncommutative and semi-Riemannian geometry. J. Geom. Phys. **56**, 175 (2006)
19. C. van den Dungen, M. Paschke, A. Rennie, Pseudo-Riemannian spectral triples and the harmonic oscillator. J. Geom. Phys. **73**, 37–57 (2013)
20. R. Verch, Quantum dirac field on Moyal-Minkowski spacetime – illustrating quantum field theory over Lorentzian spectral geometry. Acta Phys. Pol. B Proc. Suppl. **4**, 267–292 (2011)

Thermal Equilibrium States for Quantum Fields on Non-commutative Spacetimes

Gandalf Lechner and Jan Schlemmer

Contents

Abstract Fully Poincaré covariant quantum field theories on non-commutative Moyal Minkowski spacetime so far have been considered in their vacuum representations, i.e. at zero temperature. Here we report on work in progress regarding their thermal representations, corresponding to physical states at non-zero temperature, which turn out to be markedly different from both, thermal representations of quantum field theory on commutative Minkowski spacetime, and such representations of non-covariant quantum field theory on Moyal Minkowski space with a fixed deformation matrix.

Keywords Quantum field theory on non-commutative spaces • Thermal equilibrium (KMS) states

Mathematics Subject Classification (2010). 81T28, 81T05, 81R60

G. Lechner (✉)
School of Mathematics, Cardiff University, Senghennydd Road, Cardiff, Wales, CF24 4AG, UK
e-mail: LechnerG@cardiff.ac.uk

J. Schlemmer
Mathematisches Institut der Westfälischen Wilhelms-Universität, Einsteinstraße 62, 48149 Münster, Germany
e-mail: Jan.Schlemmer@math.uni-muenster.de

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_10

1 Introduction

Quantum field theory on "non-commutative spaces" [17] has been pursued in the past years for a number of reasons: On the one hand, it is generally expected that our picture of spacetime as a "classical" Lorentzian manifold, with matter described by quantum fields that propagate on this spacetime, breaks down at extremely small scales of the order of the Planck length $\lambda_P \sim 10^{-35}$ m. One expects that localization measurements resolving such scales should not be possible [15], and no sharp distinction between "matter" and "geometry" degrees of freedom should exist in this regime. Since a "quantized" space with non-commuting coordinates, say $X_1, \ldots, X_{d-1}$ (modeled as self-adjoint elements of some *-algebra) automatically yields uncertainty relations, i.e. lower bounds on products of uncertainties $\Delta_\omega X_\mu \cdot \Delta_\omega X_\nu$, QFT on non-commutative spaces naturally leads to models in which sharp joint measurements of several space-time coordinates is impossible.

Another motivation to consider such theories comes from renormalization theory: Since localization at sharp points is impossible in non-commutative spaces, one expects the ultraviolet divergences of QFT to be softer in such a setting than in usual "commutative" Minkowski space (see, for example, [24, 33]).

Non-commutative QFT models also play a prominent role in the spectral formulation of the standard model (see [10–12, 14] for just some sample articles), or in approaches to quantum gravity via non-commutative structures [36].

Furthermore, also certain low-energy limits of string theory result in field theories QFT on non-commutative spaces [13, 34], providing further motivation to study such models.

Finally, one can also take the point of view that the study of QFT on non-commutative spaces can lead to new insights about QFT on commutative spaces [8]. Independent of the motivation, there is one type of non-commutative structure which is by far the simplest and best studied one, namely Moyal-Weyl space. Here one postulates selfadjoint coordinate operators[1] X_0, X_1, X_2, X_3, subject to the canonical commutation relations

$$\big[X_\mu, X_\nu\big] = i\,\theta_{\mu\nu} \cdot 1\,, \tag{1}$$

where 1 denotes the identity element of the algebra generated by the X_μ, and the constants $\theta_{\mu\nu}$ form a real skew symmetric (4×4)-matrix. Such commutation relations are, of course, well known from the Schrödinger representation of quantum mechanics. In that situation, the X_μ correspond to position and momentum operators, and θ is given by a factor of $\hbar$ and the classical Poisson brackets.

In the setting of Moyal-Weyl *spacetime*, however, the interpretation of the X_μ is that of spatial (X_1, X_2, X_3) respectively time (X_0) coordinates (instead of coordinates

[1] For the sake of simplicity, we will stick to the physically most interesting case of $d = 4$ spacetime dimensions. With minor modifications, our considerations also apply in general dimension $d \geq 2$.

of phase space), defining a non-commutative version of Minkowski spacetime. The matrix θ is a measure for the strength of non-commutative effects, and can be taken to be proportional to λ_P^2.

This new view of the commutation relations (1) immediately leads to a well-known problem: The symmetries of (1) do not match the Poincaré symmetry of "classical" Minkowski space. Whereas translations, implemented by $X_\mu \mapsto X_\mu + x_\mu \cdot 1$ with $x \in \mathbb{R}^4$, do leave (1) invariant, the same is not true for Lorentz transformations $X_\mu \mapsto \Lambda_\mu{}^\nu X_\nu$. Only those Lorentz transformations that fix the matrix θ also respect the relation (1), thus breaking Lorentz symmetry down to a subgroup unless $\theta = 0$.

There are three different ways to deal with this situation, all of which have been considered in the literature. We recall them here and list a few sample publications for each approach.

First, one can simply accept the breaking of Lorentz symmetry, and work with models with less symmetry than their counterparts on commutative Minkowski space, see for example [23, 28]. As a second option, one can modify the commutation relations (1) in such a way that they become fully covariant. This point of view has in particular been put forward by Doplicher, Fredenhagen, and Roberts [16], who replaced the constant matrix θ by an operator-valued matrix Q in the center of the algebra generated by the X_μ, which has a full Lorentz orbit of real, Lorentz skew symmetric[2] (4×4)-matrices,

$$\Theta = \{\Lambda\theta_0\Lambda^{-1} \,:\, \Lambda \in \mathcal{L}\}\,, \tag{2}$$

as the joint spectrum of its components. Here θ_0 serves to fix the particular orbit. See also [21, 22] for other covariant models. Third, using methods from quantum groups, one can "twist" the action of the Lorentz group in such a way that it is compatible with (1) [9, 19, 39]. However, this approach is often equivalent to the previous one [31].

In this article, we will consider the fully Poincaré covariant model proposed in [21], with the aim to understand its behavior *at finite temperature*. As in the approach taken in [16], this model involves a Lorentz orbit Θ (2), but differs in its localization properties. To briefly introduce the model (more details will be provided in the following section), consider the free scalar Klein-Gordon field ϕ on Fock space $\mathcal{H}$ (i.e., in its vacuum representation, at zero temperature), and coordinate operators X_μ satisfying (1) for fixed θ, realized on a "coordinate Hilbert space" $\mathcal{V}$. On the tensor product space $\mathcal{H} \otimes \mathcal{V}$, consider the field

$$\phi_\theta^\otimes(x) = (2\pi)^{-2} \int dp\, \tilde{\phi}(p) \otimes e^{ip\cdot(X+x)}\,. \tag{3}$$

[2]Starting from this point on, we will use the Lorentz skew symmetric matrices $\vartheta_\nu^\mu = \eta^{\mu\kappa}\theta_{\kappa\nu}$ instead of the Euclidean skew symmetric ones and again denote them by θ.

There exists a natural vacuum state on the algebra generated by the (smeared) field operators $\phi_\theta^{\otimes}$, and when one passes to its GNS representation, one finds an equivalent field operator ϕ_θ, acting on Fock space $\mathcal{H}$ instead of $\mathcal{H} \otimes \mathcal{V}$ (see Sect. 2). Concretely, this amounts to replacing the usual scalar free field $\tilde{\phi}(p)$ (in momentum space) by its "twisted" version

$$\tilde{\phi}_\theta(p) = \tilde{\phi}(p) \cdot e^{-\frac{i}{2} p \cdot \theta P}, \tag{4}$$

where $P = (P_0, P_1, P_2, P_3)$ denote the energy momentum operators on Fock space (see also [3]).

When understood in a proper distributional sense, the construction (4) is unitarily equivalent to the one on $\mathcal{V} \otimes \mathcal{H}$ for fixed θ [21], but there is one big advantage: Fields for different θ are represented on the same Hilbert space and, since $\mathcal{H}$ is the usual Fock space of the Klein-Gordon field, one has a unitary representation U of the full Poincaré group. Adjoint action with $U(a, \Lambda)$ on a field operator ϕ_θ yields $\phi_{\Lambda\theta\Lambda^{-1}}$ (which is compatible with (1)) but more importantly, is another well-defined field operator on the same Hilbert space $\mathcal{H}$. It is thus possible to make the theory covariant, by not just taking field operators ϕ_θ for some fixed θ, but instead ϕ_θ for all θ from an orbit Θ (2).

The model we want to consider is then described by the field algebra $\mathcal{P}_\Theta$ of all polynomials in (smeared) field operators $\phi_\theta(f)$, where θ runs over the Lorentz orbit Θ, and f over the space of all test functions $\mathscr{S}(\mathbb{R}^4)$. We also include the identity operator 1, so that $\mathcal{P}_\Theta$ has the structure of a unital *-algebra.

In this contribution, we want to discuss thermal equilibrium states for this model as a concrete representative of a quantum field theory on a non-commutative spacetime. Below we list our motivations for this investigation and some of the questions we want to address.

(Q1). An important selection criterion for physically meaningful theories is their ability to allow for thermal states. "Does the considered model have thermal equilibrium states?", the basic question preceding any analysis of thermal behavior, will be investigated here. At first sight, the appearance of functions of the energy-momentum operators P_μ in the field algebra (already anticipated in the twisted field operators (4)) seems to threaten this. Further investigation however shows that things are more complicated, warranting a more detailed study.

(Q2). On scales accessible to us, QFT on non-commutative spaces can be expected to yield only tiny deviations from the predictions of usual QFT. However, it is not very clear what these deviations are, or how they could be observed. In the model at hand, the effect of the noncommutativity parameter θ on scattering processes (at zero temperature) was investigated in [21], and shown to lead to modifications in the phase shift of two-particle scattering. Here we ask in the same model "what are the observational consequences of a non-commutative structure of spacetime on the thermal behavior?"

(Q3). The model under consideration can also be considered as a "deformed" theory of fields on ordinary Minkowski spacetime, where the fields are however only localized in spacelike wedge regions. This observation is in line with several investigations of deformations of quantum field theories which are compatible with Poincaré covariance and (at least partial) localization/causality properties [38, Sect. 6],[29]. It is a common theme of these approaches that they make use of a condition of positivity of the energy. Such a spectrum condition holds in vacuum representations of QFT, where the vacuum state is a ground state for the energy, but not in thermal representations because of the presence of a heat bath from which arbitrary amounts of energy can be extracted. In fact, typical deformation schemes do not lead to wedge-locality when considering thermal field theory instead of QFT in its vacuum representation [30].

From the point of view of deformation theory, it is interesting to ask what one can do without the spectrum condition. As we shall see, an analysis of thermal representations of deformed vacuum field theories, such as the one considered here, can shed new light onto this question.

On a mathematical level, these questions turn out to be best analyzed with *algebraic methods*. As appropriate for proceedings of a conference covering a wide range of topics, we will next outline the tools we rely on, essentially reviewing the formalism of KMS states on unital *-algebras (see, for example, [4]).

Following standard procedure in quantum physics [18], *states* on the field (or observable) algebra are modeled as certain functionals $\omega : \mathcal{P}_\Theta \to \mathbb{C}$, mapping field polynomials, generically denoted $F \in \mathcal{P}_\Theta$, to their expectation values $\omega(F)$. These functionals are taken to be linear, normalized in the sense that $\omega(1) = 1$, and *positive*. The precise definition of positivity depends a little on the topological structure of the algebra,[3] but always involves the condition that "squares" F^*F should have positive expectation values,

$$\omega(F^*F) \geq 0\,, \qquad F \in \mathcal{P}_\Theta\,, \tag{5}$$

which is necessary for ω to have a probability interpretation (positive uncertainties).

In our model, a simple example of such a state is the vacuum state on $\mathcal{P}_\Theta$: As $\mathcal{P}_\Theta$ consists of operators on the Fock space $\mathcal{H}$ containing the (normalized) vacuum vector Ω, the vacuum state is $\omega_{\text{vac}}(F) = \langle \Omega\,, F\Omega \rangle$.

However, the concept of state is not restricted to vector states, and thinking of thermal equilibrium states in quantum mechanics, one might consider states of the Gibbs form $\omega_\beta(F) = Z^{-1}\text{Tr}(F\, e^{-\beta H})$, where $H = P_0$ is the Hamiltonian, $\beta = 1/T$ the inverse temperature, and $Z = \text{Tr}(e^{-\beta H})$ the partition function. Such Gibbs ensembles are well-defined in finite volume, where the Hamiltonian has discrete

[3] Usually, one also requires states to be continuous. In the case of a C^*-algebra, continuity is a consequence of positivity, but for more general topological algebras such as the field algebra considered here, this is not the case. For the sake of simplicity, we do not go into these details here.

spectrum and the trace exists. In the case of a theory in infinite volume, such as the one considered here, Gibbs states do however not exist per se, but rather only as quantities approximating the equilibrium states in infinite volume (thermodynamic limit).

It is long since known [25] that a more intrinsic formulation of thermodynamic equilibrium states can be given in terms of the Kubo-Martin-Schwinger (KMS) condition. This condition trades the explicit Gibbs form of the state for a boundary condition, involving analytic continuation along the Heisenberg dynamics

$$\tau_t(F) := e^{itP_0} F e^{-itP_0} . \tag{6}$$

The precise definition of the KMS property again depends a little on the topological structure of the algebra [20], but always involves the following condition (which is sufficient in the case of a C^*-algebra, and to which we restrict here for the sake of simplicity). A *KMS state at inverse temperature* $\beta > 0$ is a state ω on $\mathcal{P}_\Theta$ which has the property that for each two field polynomials $F, G \in \mathcal{P}_\Theta$, the function

$$f_{F,G}(t) := \omega(F\tau_t(G)) , \qquad t \in \mathbb{R} , \tag{7}$$

has an analytic continuation to the complex strip $\mathbb{R} + i(0, \beta)$, is bounded and continuous on the closed strip $\mathbb{R} + i[0, \beta]$, and satisfies the boundary condition

$$f_{F,G}(t + i\beta) = \omega(\tau_t(G)F) , \qquad t \in \mathbb{R}. \tag{8}$$

KMS states show the typical features of thermal equilibrium states in general, such as invariance under the dynamics, stability, and passivity [4]. For states on "type I von Neumann factors" [4], as they are encountered in quantum mechanics, and dynamics with a Hamiltonian H such that $\mathrm{Tr}(e^{-\beta H})$ exists, the KMS states coincide with the Gibbs states. Thus the KMS condition provides a good characterization of thermal equilibrium. Returning to our above list of questions, the first question (Q1) can therefore be phrased as the question about existence of KMS states on $\mathcal{P}_\Theta$. Explicit knowledge of such states (say, in terms of its n-point functions) is also the basis of a quantitative understanding of the thermodynamic behavior of the considered system (question (Q2)). In the present conference paper, we restrict ourselves to announce several results concerning the algebraic structure of $\mathcal{P}_\Theta$ and its equilibrium states, including explicit formulas for their n-point functions. A full analysis with detailed proofs will be presented elsewhere. We however wish to motivate why it is useful to have a closer look at the algebraic structure of $\mathcal{P}_\Theta$ in this context, and to this end, proceed with an outline of the paper.

In Sect. 2, we introduce the vacuum representation of the model in more detail. The algebra $\mathcal{P}_\Theta$, containing smeared polynomials in all field operators ϕ_θ, $\theta \in \Theta$, obviously has as subalgebras the polynomials in fields ϕ_θ with a *fixed* $\theta \in \Theta$. These subalgebras will be denoted $\mathcal{P}_{\{\theta\}} \subset \mathcal{P}_\Theta$, and referred to as "fibers". Since each such fiber is invariant under the dynamics τ_t, it is clear that given a KMS state on $\mathcal{P}_\Theta$, it

restricts to KMS states on each of the fibers $\mathcal{P}_{\{\theta\}}$. Thus, as a preliminary step, we consider in Sect. 3 the KMS states on a fixed fiber.

It turns out that the thermal states of $\mathcal{P}_{\{\theta\}}$ can be easily analyzed completely. Namely, by exploiting a natural bijection with the "zero fiber" $\mathcal{P}_{\{0\}}$, containing the polynomials in the undeformed free Klein-Gordon field, we find that the KMS states on $\mathcal{P}_{\{\theta\}}$ and $\mathcal{P}_{\{0\}}$ are in one to one correspondence. Moreover, one can explicitly calculate all n-point functions of these equilibrium states by basically the same techniques as in the undeformed case. These results are obtained by making use of the machinery underlying Rieffel's deformation theory [32] and the related concept of warped convolutions [7, 8], and allow us to substantially generalize findings of Balachandran and Govindarajan about the thermal four-point function at fixed noncommutativity θ [2].

Having settled the structure of thermal equilibrium states at fixed θ (i.e., for the non-covariant models build on (1)), we proceed to the analysis of thermal equilibrium states on the full field algebra $\mathcal{P}_\Theta$ in Sect. 4. Here a completely new aspect enters, both on the level of the structure of the field algebra, and on the level of its thermal equilibrium states. To see this effect, note that the field operators[4] (4) satisfy the twisted commutation relation

$$\tilde{\phi}_\theta(p)\tilde{\phi}_{\theta'}(p') - e^{ip\cdot(\theta+\theta')p'}\,\tilde{\phi}_{\theta'}(p')\tilde{\phi}_\theta(p) = \tilde{C}(p,p')\,e^{ip\cdot(\theta-\theta')P}\,, \tag{9}$$

where $\tilde{C}(p,p')$ denotes the (number-valued) momentum space commutator of two undeformed fields $\tilde{\phi}(p), \tilde{\phi}(p')$. For $\theta, \theta' \in \Theta$, $\theta \neq \theta'$, this shows that certain functions of the energy momentum operators P_μ are elements of $\mathcal{P}_\Theta$ (which are not present in the fibers $\mathcal{P}_{\{\theta\}}$). In addition to the fibers $\mathcal{P}_{\{\theta\}}$, the algebra thus also contains a commutative subalgebra $\mathcal{T}_\Theta$ containing functions of P.

This subalgebra has the peculiar property that, consisting of functions of the (commuting) energy momentum operators $P_0, \ldots, P_3$, each of its elements is invariant under the dynamics $\tau_t(F) = e^{itP_0}Fe^{-itP_0}$.

Thus the functions $f_{F,G}(t) = \omega(F\tau_t(G))$ appearing in the KMS condition are *constant* for each $F, G \in \mathcal{T}_\Theta$, and because $\mathcal{T}_\Theta$ is abelian, ω automatically satisfies the required analyticity and boundary condition (8). This observation implies that, in sharp contrast to the situation on the fibers $\mathcal{P}_{\{\theta\}}$, *each* state on $\mathcal{T}_\Theta$ is a KMS state. In other words, the KMS condition does not put any constraints on the expectation values $\omega(F)$, $F \in \mathcal{T}_\Theta$.

As a consequence, a very large family of KMS functionals (at fixed temperature) appears. Usually, the appearance of several distinct KMS states at the same temperature is taken as a sign for different thermodynamic phases that can coexist at that temperature. The picture of many "non-commutative phases" appearing at any finite temperature seems to be hard to maintain, and in fact, it has to be taken into account that these KMS functionals must also meet the essential positivity

[4]Here and in the following, we adopt the convention to rescale θ by a factor $\frac{1}{2}$ to obtain simpler formulas.

condition (5) in order to have physical meaning. While on the level of linear relations used to determine n-point functions, there are many similarities to thermal states of free field models – with the exception of the mentioned additional freedom on $\mathcal{T}_\Theta$ – things get more complicated for the nonlinear relation (5).

Using yet another subalgebra $\mathcal{J}_\Theta \subset \mathcal{P}_\Theta$, namely an ideal generated by the projection onto the vacuum vector, the positivity questions can be completely settled. It turns out that the positivity requirement singles out a *unique* KMS state on $\mathcal{P}_\Theta$. We discuss some of its properties in Sect. 4. In particular, we describe its associated GNS representation, which is "more commutative" than the algebra $\mathcal{P}_\Theta$ at temperature zero. We end by explaining the implications of this observation for the question (Q3) on our list, and with an account of some open questions which we are currently investigating.

2 The Model

In this section we define the vacuum representation of the model that we consider.

Fixing a mass parameter $m > 0$, we consider the single-particle Hilbert space

$$\mathcal{H}_1 := L^2(\mathbb{R}^4, d\mu_m(p)),$$

with the mass shell measure $d\mu_m(p) = \delta(p^0 - \epsilon(\mathbf{p}))\, \frac{d^4p}{2\epsilon(p)}$, where $p = (p^0, \mathbf{p})$ and $\epsilon(\mathbf{p}) = (m^2 + \mathbf{p}^2)^{1/2}$ is the single particle Hamiltonian. On $\mathcal{H}_1$ there acts the unitary irreducible representation U_1 of the proper orthochronous Poincaré group with mass m and spin zero, given by $(U_1(a, \Lambda)\psi)(p) = e^{ip\cdot a}\psi(\Lambda^{-1}p)$.

The full vacuum Hilbert space $\mathcal{H}$ is defined as the Bose Fock space over $\mathcal{H}_1$. It carries the second quantized representation U of the Poincaré group and contains the U-invariant vacuum vector Ω. For pure translation operators, we will also write

$$U(x) = e^{ix\cdot P} \equiv U(x, 1)\,, \qquad x \in \mathbb{R}^4\,. \tag{10}$$

Here $P = (P_0, P_1, P_2, P_3)$ are the energy-momentum operators (with joint spectrum contained in the forward light cone). In particular, $P_0 = H$ is the Hamiltonian giving the dynamics with respect to which we will be looking for thermal equilibrium.

The adjoint action of U on operators will, as usual, be denoted $\alpha_{x,\Lambda}(F) = U(x, \Lambda)FU(x, \Lambda)^{-1}$, and for the dynamics (time translations), we reserve the shorter notation

$$\tau_t(F) := e^{itH}Fe^{-itH} = \alpha_{(t,0,0,0),1}(F)\,. \tag{11}$$

On $\mathcal{H}$, the (undeformed) free scalar Klein-Gordon field ϕ of mass m acts in the usual manner, i.e.

$$\phi(f) = a^\dagger(\tilde{f}) + a(\bar{\tilde{f}})$$

with $a, a^\dagger$ Bose creation and annihilation operators, $f \in \mathscr{S}(\mathbb{R}^4)$ a test-function from Schwartz space and $f \mapsto \tilde{f}$ the Fourier transform. We will often write ϕ in terms of its distributional kernels in momentum space, i.e.

$$\phi(f) = \int d^4p\, \tilde{\phi}(p)\tilde{f}(-p)\,. \tag{12}$$

Well-known properties of ϕ that are relevant here are first of all its c-number commutation relations

$$[\tilde{\phi}(p), \tilde{\phi}(q)] = \delta(p+q)\,\epsilon(p^0)\,\delta(p^2+m^2)\cdot 1 =: \tilde{C}(p,q)\cdot 1\,, \tag{13}$$

which imply in particular *locality*, that is $[\phi(x), \phi(y)] = 0$ for x spacelike to y.

Furthermore, ϕ transforms covariantly under the representation U, i.e.

$$U(a,\Lambda)\tilde{\phi}(p)U(a,\Lambda)^{-1} = e^{ip\cdot a}\cdot\tilde{\phi}(\Lambda p)\,. \tag{14}$$

According to the terminology used in the Introduction, the field algebra of the free field ϕ is denoted $\mathcal{P}_{\{0\}}$, because it corresponds to fixed deformation parameter $\theta = 0$. Since we are interested in QFT at finite temperature, we also recall the known results about the KMS states of $\mathcal{P}_{\{0\}}$.

Lemma 2.1

(a) There exists a unique[5] *KMS state ω_0 on $\mathcal{P}_{\{0\}}$.*
(b) ω_0 is translationally invariant, i.e. $\omega_0 \circ \alpha_{x,1} = \omega_0$ for all $x \in \mathbb{R}^4$.
(c) If φ is a KMS functional[6] *on $\mathcal{P}_{\{0\}}$, then there exists $c \in \mathbb{C}$ such that $\varphi = c\cdot\omega_0$.*

Item (2.1) tells us that the linear relations already fix the state up to normalization, so the problem of determining KMS states is essentially a linear one.

Explicitly, ω_0 can be described by its n-point functions, which are of quasi-free form. Denoting the distributional kernels of $f_1 \otimes \ldots \otimes f_n \mapsto \omega_0(\phi(f_1)\cdots\phi(f_n))$ (in momentum space) by $\tilde{\omega}_{0,n}(p_1,\ldots,p_n)$, we have the formulas, $n \in \mathbb{N}_0$,

$$\tilde{\omega}_{0,2n+1}(p_1,\ldots,p_{2n+1}) = 0, \tag{15}$$

$$\tilde{\omega}_{0,2n}(p_1,\ldots,p_{2n}) = \sum_{(\mathbf{l},\mathbf{r})}\prod_{j=1}^{n}\tilde{\omega}_{0,2}(p_{l_j},p_{r_j}) \qquad \tilde{\omega}_{0,2}(p,q) = \frac{\tilde{C}(p,q)}{1-e^{\beta p^0}}. \tag{16}$$

[5] "Unique" refers to fixed inverse temperature $\beta > 0$, and fixed dynamics τ (11). Furthermore, for the *-algebraic setting considered here, some weak continuity assumptions are required in order to have analytical tools like Fourier transforms available. Here and in the following we will always restrict to states whose n-point functions are temperate distributions.

[6] That is, a linear functional which satisfies the KMS condition, but is not necessarily normalized or positive.

Here the sum runs over all *contractions* $(\mathbf{l}, \mathbf{r})$ of $\{1, \ldots, 2n\}$, i.e. sets of ordered multi indices $\mathbf{l} = (l_1, \ldots, l_n)$, $\mathbf{r} = (r_1, \ldots, r_n)$ such that $l_1 < \ldots < l_n$, $l_k < r_k$, $k = 1, \ldots, n$, and $\{l_1, \ldots, l_n, r_1, \ldots, r_n\} = \{1, \ldots, 2n\}$.

Regarding (b), recall that any KMS state is invariant under the time translations τ it refers to, but not necessarily invariant under spatial translations as well. It is clear from (16) and (13) that ω_0 is also invariant under spatial rotations (but not under Lorentz boosts). However, the only relevant symmetry of ω_0 that we will exploit later is its invariance under spacetime translations.

We also recall the GNS representation of $\mathcal{P}_{\{0\}}$ with respect to its KMS state ω_0, the well-known Araki-Woods representation [1]: The representation Hilbert space is[7] $\mathcal{H}_0 := \mathcal{H} \otimes \overline{\mathcal{H}}$, the vector implementing the KMS state is $\Omega_0 := \Omega \otimes \overline{\Omega}$, and the vacuum fields $\phi(f) \in \mathcal{P}_{\{0\}}$ are represented on $\mathcal{H}_0$ as $\pi_0(\phi(f)) = \phi((1 + \rho)^{1/2} f) \otimes \overline{1} + 1 \otimes \overline{\phi(\rho^{1/2} f)}$, where ρ acts in momentum space by multiplying with $p \mapsto (e^{\beta\epsilon(\mathbf{p})} - 1)^{-1}$. These data form the GNS triple of $(\mathcal{P}_{\{0\}}, \omega_0)$, i.e.

$$\omega_0(F_0) = \langle \Omega_0, \pi_0(F_0)\Omega_0 \rangle_{\mathcal{H}_0}\,, \qquad F_0 \in \mathcal{P}_{\{0\}}\,. \tag{17}$$

As ω_0 is invariant under translations, $\mathcal{H}_0$ also carries a unitary representation U_0 of the space-time translations, related to the translations U in the vacuum representation by $U_0(x) = U(x) \otimes \overline{U(x)}$. Because of the conjugation in the second tensor factor, this representation does not have positive energy, but rather all of $\mathbb{R}^4$ as its energy-momentum spectrum.

Having recalled the relevant structures of the undeformed free field theory, we now proceed to its deformed version. Let θ denote a real Lorentz skew symmetric (4×4)-matrix, and define

$$\tilde{\phi}_\theta(p) := \tilde{\phi}(p)\, U(-\theta p)\,. \tag{18}$$

Since $U(0) = 1$, this definition returns the original field $\phi_0 = \phi$ for $\theta = 0$.

The definition (18) has to be understood in the sense of distributions. For a proper definition in terms of test functions, consider the expressions

$$(f_1, \ldots, f_n) \mapsto \Psi_n(f_1 \otimes \ldots \otimes f_n) := \phi(f_1) \cdots \phi(f_n)\Omega\,,$$

which define vector-valued distributions $\Psi_n : \mathscr{S}(\mathbb{R}^{4n}) \to \mathcal{H}$, $n \in \mathbb{N}_0$, and the linear span $\mathcal{D}$ of all their ranges is a dense subspace of $\mathcal{H}$ [37]. In particular, Ψ_n extends to all test functions of $4n$ variables, also those which are not of product form. The deformed field operator $\phi_\theta(f)$, smeared with a test function $f \in \mathscr{S}(\mathbb{R}^4)$, can then be defined on $\mathcal{D}$ as [22, 35]

$$\phi_\theta(f)\Psi_n(g_n) := \Psi_{n+1}(f \otimes_\theta g_n), \qquad g_n \in \mathscr{S}(\mathbb{R}^{4n}),\ n \in \mathbb{N}_0, \tag{19}$$

[7] $\overline{\mathcal{H}}$ denotes the conjugate of the vacuum Fock space $\mathcal{H}$.

where the twisted tensor product $f \otimes_\theta g_n$ is given in Fourier space by

$$\widetilde{(f \otimes_\theta g_n)}(p, q_1, \ldots, q_n) := \prod_{r=1}^{n} e^{ip\cdot\theta q_r} \tilde{f}(p) \cdot \tilde{g}_n(q_1, \ldots, q_n). \tag{20}$$

The properties of ϕ are affected by the deformation $\phi \rightsquigarrow \phi_\theta$. Regarding covariance, one finds by straightforward calculation the modified transformation law

$$U(a, \Lambda)\tilde{\phi}_\theta(p)U(a, \Lambda)^{-1} = e^{ia\cdot p}\, \tilde{\phi}_{\Lambda\theta\Lambda^{-1}}(\Lambda p)\,, \tag{21}$$

which states that translations are still a symmetry of the deformed fields at fixed θ, but Lorentz transformations in general change the deformation parameter (cf. the discussion of the Weyl-Moyal relations in the Introduction). Also note that ϕ_θ is not local if $\theta \neq 0$. However, certain remnants of locality are still present after the deformation. Comparing ϕ_θ with the inversely deformed field $\phi_{-\theta}$, one finds localization in Rindler wedges. We refer to [21] for more details on this, and the consequences for two-particle scattering.

Denoting the algebra of all polynomials in (smeared) field operators $\phi_\theta(f)$ (with fixed θ) by $\mathcal{P}_{\{\theta\}}$, the transformation law (21) yields

$$\alpha_{x,\Lambda}(\mathcal{P}_{\{\theta\}}) = \mathcal{P}_{\{\Lambda\theta\Lambda^{-1}\}}\,. \tag{22}$$

We therefore enlarge our field algebra to contain $\mathcal{P}_{\{\Lambda\theta\Lambda^{-1}\}}$ for all Lorentz transformations Λ in order to arrive at a fully covariant model theory.

Definition 2.2 Let $\Theta = \{\Lambda\theta_0\Lambda^{-1} \mid \Lambda \in \mathcal{L}_+^\uparrow\}$ be the orbit of some reference matrix $\theta_0 \in \mathbb{R}_-^{4\times 4}$ under the Lorentz group $\mathcal{L}_+^\uparrow$. Then $\mathcal{P}_\Theta$ is defined as the *-algebra generated by all $\mathcal{P}_{\{\theta\}}$, $\theta \in \Theta$. The *-subalgebras $\mathcal{P}_{\{\theta\}} \subset \mathcal{P}_\Theta$, $\theta \in \Theta$, will be referred to as the fibers (over θ) of $\mathcal{P}_\Theta$.

This *-algebra of unbounded operators is the starting point for our analysis of thermal states in the following sections.

3 KMS States for the Fiber Algebras

Given any KMS state on the full field algebra $\mathcal{P}_\Theta$, one obtains KMS states on all of its fibers $\mathcal{P}_{\{\theta\}} \subset \mathcal{P}_\Theta$, $\theta \in \Theta$, by restriction. In this section, we therefore consider the KMS states of the fiber algebras $\mathcal{P}_{\{\theta\}}$ as a first step towards understanding the KMS states of $\mathcal{P}_\Theta$. This amounts to determining the thermal equilibrium states of QFT models without Lorentz covariance, formulated on Moyal space with fixed θ.

The analysis of thermal states on $\mathcal{P}_{\{\theta\}}$ becomes most transparent if one uses the fact that $\mathcal{P}_{\{\theta\}}$ can be seen as a *deformation* of the "zero fiber" $\mathcal{P}_{\{0\}}$ (the field

algebra of the Klein Gordon field on commutative Minkowski spacetime), related to introducing a new product on $\mathcal{P}_{\{0\}}$.

This situation is familiar from deformation quantization, where one introduces (non-commutative) star products on the (initially commutative) algebra of classical observables by pulling back the operator product of the quantum observables. In fact, since the commutation relations (1) are just the Heisenberg commutation relations, it is no surprise that there are several mathematical analogies between theories on Moyal space with a fixed non-commutativity matrix θ on the one hand, and deformation quantization on the other hand. In the present setting, where also the algebra $\mathcal{P}_{\{0\}}$ corresponding to the undeformed situation is non-commutative, the right tools for setting up such a deformation are Rieffel's procedure [32] and its generalizations, in particular the "warped convolution" [7, 8]. We briefly recall here the relevant structures.

To begin with, we introduce the "Weyl-Moyal tensor product" between test functions of several variables as a slight generalization of (20). For $f_n \in \mathscr{S}(\mathbb{R}^{4n})$, $g_m \in \mathscr{S}(\mathbb{R}^{4m})$, we define

$$\widetilde{(f_n \otimes_\theta g_m)}(p_1, \ldots, p_n; q_1, \ldots, q_m) := \prod_{l=1}^{n} \prod_{r=1}^{m} e^{ip_l \cdot \theta q_r} \cdot \tilde{f}_n(p_1, \ldots, p_n)\, \tilde{g}_m(q_1, \ldots, q_m)\,. \tag{23}$$

This associative product on the tensor algebra over $\mathscr{S}(\mathbb{R}^4)$ induces a new, "deformed" product $\times_\theta$ between field operators. Setting

$$\phi(f_n) := \int d^{4n}x f_n(x_1, \ldots, x_n)\, \phi(x_1) \cdots \phi(x_n) \tag{24}$$

for test functions $f_n \in \mathscr{S}(\mathbb{R}^{4n})$ of n variables, we define

$$\phi(f_n) \times_\theta \phi(g_m) := \phi(f_n \otimes_\theta g_m)\,. \tag{25}$$

This product is an adaptation of Rieffel's product [32] to field algebras as they appear in Wightman QFT [22]. Equipping the zero fiber $\mathcal{P}_{\{0\}}$ with the product $\times_\theta$ instead of its original product (the usual operator product, which for field operators corresponds to the normal tensor product between test functions) results in a deformed version of $\mathcal{P}_{\{0\}}$: The linear structure is the same as that of $\mathcal{P}_{\{0\}}$, and thanks to $(F_0 \times_\theta G_0)^* = G_0^* \times_\theta F_0^*$ and $F_0 \times_\theta 1 = 1 \times_\theta F_0 = F_0$, $F_0, G_0 \in \mathcal{P}_{\{0\}}$, also the identity and star involution of $\mathcal{P}_{\{0\}}$ are unchanged [22, 32]. We write $(\mathcal{P}_{\{0\}}, \times_\theta)$ when we want to emphasize that we consider the vector space $\mathcal{P}_{\{0\}}$ equipped with the product $\times_\theta$.

To formulate the relation between $(\mathcal{P}_{\{0\}}, \times_\theta)$ and the fiber $\mathcal{P}_{\{\theta\}}$ over $\theta \in \mathbb{R}^{4\times 4}_-$, we introduce the "warped convolution" map $D_\theta : \mathcal{P}_{\{0\}} \to \mathcal{P}_{\{\theta\}}$, which is defined on the generating fields by

$$D_\theta(\phi(f_n)) := \phi_\theta(f_n), \qquad f_n \in \mathscr{S}(\mathbb{R}^{4n}), \tag{26}$$

where $\phi_\theta(f_n)$ is defined as in (24), with ϕ replaced by ϕ_θ, and then extended by linearity.

Proposition 3.1 *The map D_θ is an isomorphism of unital *-algebras between the zero fiber $(\mathcal{P}_{\{0\}}, \times_\theta)$, with the product $\times_\theta$, and the fiber $\mathcal{P}_{\{\theta\}}$ over θ, with the usual operator product. That is, D_θ is a linear bijection satisfying for $F_0, G_0 \in \mathcal{P}_{\{0\}}$,*

(a) $D_\theta(F_0 \times_\theta G_0) = D_\theta(F_0)D_\theta(G_0)$.
(b) $D_\theta(1) = 1$.
(c) $D_\theta(F_0^*) = D_\theta(F_0)^*$.

Moreover, D_θ commutes with translations, i.e.

$$\alpha_{x,1} \circ D_\theta = D_\theta \circ \alpha_{x,1}\,, \qquad x \in \mathbb{R}^4\,. \tag{27}$$

We mention as an aside that just like $\mathcal{P}_{\{0\}}$, also $\mathcal{P}_{\{\theta\}} = D_\theta(\mathcal{P}_{\{0\}})$ has the vacuum vector Ω as a cyclic vector because $D_\theta(F_0)\Omega = F_0\Omega$, $F_0 \in \mathcal{P}_{\{0\}}$ [8].

Since $(\mathcal{P}_{\{0\}}, \times_\theta)$ and $\mathcal{P}_{\{0\}}$ coincide as vector spaces, it is straightforward to pass from linear[8] functionals on $\mathcal{P}_{\{0\}}$ to functionals on $(\mathcal{P}_{\{0\}}, \times_\theta)$: One can simply use the *same* functional. Formulated in terms of $\mathcal{P}_{\{\theta\}} = D_\theta(\mathcal{P}_{\{0\}})$, this means that a functional $\omega : \mathcal{P}_{\{0\}} \to \mathbb{C}$ is transported to a functional $\omega_\theta : \mathcal{P}_{\{\theta\}} \to \mathbb{C}$, defined as

$$\omega_\theta := \omega_0 \circ {D_\theta}^{-1}\,. \tag{28}$$

This definition yields a one to one correspondence between functionals on the undeformed fiber $\mathcal{P}_{\{0\}}$ and the deformed fiber $\mathcal{P}_{\{\theta\}}$. For $\theta = 0$, one recovers the original functional $\omega_0 = \omega$.

In view of Proposition 3.1, the correspondence (28) preserves normalization and invariance under translations, i.e. $\omega_\theta(1) = 1$ if and only if $\omega_0(1) = 1$, and $\omega_\theta \circ \alpha_{x,1} = \omega_\theta$ for all $x \in \mathbb{R}^4$ if and only if $\omega_0 \circ \alpha_{x,1} = \omega_0$ for all $x \in \mathbb{R}^4$.

We are interested in KMS states, and therefore also have to consider the compatibility of the map $\omega \mapsto \omega_\theta$ with positivity, and with the KMS condition. The notion of positivity is a different one in $\mathcal{P}_{\{0\}}$ and $(\mathcal{P}_{\{0\}}, \times_\theta)$: Whereas squares of the form $F_0^*F_0$ are positive in the sense of $\mathcal{P}_{\{0\}}$, squares of the form $F_0^* \times_\theta F_0$ are positive in the sense of $(\mathcal{P}_{\{0\}}, \times_\theta)$. These two positive cones do not coincide, and therefore a positive functional ω on $\mathcal{P}_{\{0\}}$ is in general not positive on $(\mathcal{P}_{\{0\}}, \times_\theta)$ [27].

However, things simplify drastically when considering *translationally invariant* functionals ω on $\mathcal{P}_{\{0\}}$. In this case, one has [22, 35]

$$\omega(F_0 \times_\theta G_0) = \omega(F_0G_0)\,, \qquad F_0, G_0 \in \mathcal{P}_{\{0\}}\,, \tag{29}$$

[8] All functionals considered here are linear, so that we refer to them just as functionals for brevity.

similar to the well-known formula $\int d^4x\,(f \star_\theta g)(x) = \int d^4x f(x)g(x)$ for the Weyl-Moyal star product. From (29) it is clear that with a translationally invariant, positive functional $\omega : \mathcal{P}_{\{0\}} \to \mathbb{C}$, also $\omega_\theta : \mathcal{P}_{\{\theta\}} \to \mathbb{C}$ is positive (at least on squares). Namely, for arbitrary $F_0 \in \mathcal{P}_{\{0\}}$, we have

$$\omega_\theta(D_\theta(F_0)^* D_\theta(F_0)) = \omega_\theta(D_\theta(F_0^* \times_\theta F_0)) = \omega(F_0^* \times_\theta F_0) = \omega(F_0^* F_0) \geq 0\,.$$

Furthermore, by the same argument one also sees that the functions

$$t \mapsto \omega_\theta(D_\theta(F)\tau_t(D_\theta(G))) = \omega(F\tau_t(G))$$

are independent of θ, so that their analyticity properties and the relation (8) between their boundary values, as required in the KMS condition, transfer from the undeformed fiber to the deformed one immediately.

All this applies only to KMS states that are invariant under all space-time translations. However, since the (unique) KMS state on $\mathcal{P}_{\{0\}}$ has this property (Lemma 2.1(b)), these considerations cover the situation of interest here. We find the following result.

Theorem 3.2

(a) The mapping $\omega_0 \mapsto \omega_\theta$ defined above is a bijection between the functionals on $\mathcal{P}_{\{0\}}$ and $\mathcal{P}_{\{\theta\}}$. The functional ω_θ is normalized (respectively translationally invariant) if and only if ω_0 is normalized (respectively translationally invariant).

(b) For translationally invariant functionals ω_0 on $\mathcal{P}_{\{0\}}$, ω_θ satisfies the KMS condition (is positive) if and only if ω_0 satisfies the KMS condition (is positive).

(c) There exists a unique KMS state on each fiber $\mathcal{P}_{\{\theta\}}$, given by $\omega_\theta = \omega_0 \circ {D_\theta}^{-1}$.

(d) The n-point functions of this unique KMS state ω_θ are

$$\tilde{\omega}_{\theta,n}(p_1,\ldots,p_n) := \omega_\theta(\tilde{\phi}_\theta(p_1)\cdots\tilde{\phi}_\theta(p_n)) = \prod_{1\leq l<r\leq n} e^{ip_l\cdot\theta p_r}\cdot\tilde{\omega}_{0,n}(p_1,\ldots,p_n). \tag{30}$$

The formula for n-point functions stated in part (d) can be derived by straightforward calculation similar to the vacuum case [22].

The KMS states ω_θ on $\mathcal{P}_{\{\theta\}}$ can also be obtained by direct calculation of their n-point functions by imposing the KMS condition (cf. the calculation at the beginning of the next section). This approach was taken in [26], see also [2] for a partial analysis in the context of non-covariant field theories on Moyal space. However, in our opinion, the more algebraic point of view taken here makes the situation particularly clear. Moreover, it applies without essential modifications also to more complicated field theories – in particular, the commutation relations (13) are not needed in our approach, but often form the basis of direct calculations.

The situation described in Theorem 3.2 closely resembles the case of undeformed fields: For each inverse temperature $\beta > 0$, there exists exactly one thermal equilibrium state, and this state is translationally invariant. Furthermore, the distributional

kernels of its n-point functions in momentum space depend on θ only via phase factors. Note however that due to these phase factors, the thermal states on $\mathcal{P}_{\{\theta\}}$ are no longer quasi-free. This close relation between $\mathcal{P}_{\{\theta\}}$ and $\mathcal{P}_{\{0\}}$ is also reflected on the level of the (GNS) representations π_θ and π_0 induced by ω_θ and ω_0: The GNS representation π_θ of $\mathcal{P}_{\{\theta\}}$ with respect to its unique KMS state $\omega_\theta = \omega_0 \circ {D_\theta}^{-1}$ acts on the same representation space $\mathcal{H}_0$ as for $\theta = 0$, with the same implementing vector Ω_0 (cf. page 188). Analogously to the vacuum case (4), the representation of the deformed fiber $\mathcal{P}_{\{\theta\}}$ can be realized as (in the sense of distributions)

$$\pi_\theta(\tilde{\phi}(p)) = \pi_\theta(\tilde{\phi}(p))U_0(-\theta p)\,. \tag{31}$$

That is, the thermal representation of a deformed fiber is given by warped convolution w.r.t. the translation representation U_0 on the thermal Hilbert space. In this sense, deforming and going to a thermal representation commute on a single fiber.

However, the algebra generated by the fields $\pi_\theta(\phi_\theta(f))$, when θ is no longer fixed but ranges over the orbit Θ, does *not* form a representation of $\mathcal{P}_\Theta$. This is so because of certain residual localization properties that are present in $\mathcal{P}_\Theta$: If the supports of two test functions f, g are carefully chosen (in spacelike wedges depending on θ), then $[\phi_\theta(f), \phi_{-\theta}(g)] = 0$ as a relation in $\mathcal{P}_\Theta$. This relation is a consequence of the spectrum condition in the vacuum case, and clearly persists in any representation of $\mathcal{P}_\Theta$. But the fields $\pi_\theta(\phi_\theta(f))$ and $\pi_{-\theta}(\phi_{-\theta}(g))$ do not commute in general for f and g with the mentioned support properties. This is a consequence of the spectrum condition being violated in the thermal representation [30].

This observation already indicates that a thermal representation of the full algebra $\mathcal{P}_\Theta$ has to take place on a "larger" space than $\mathcal{H}_0$, such that more elements have the possibility to commute. How this representation, induced by a state with many vanishing n-point functions, comes about, will be the topic of the next and final section.

4 KMS States for the Covariant Theory

After discussing KMS states for the fiber subalgebras $\mathcal{P}_{\{\theta\}} \subset \mathcal{P}_\Theta$ of our field algebra, we now come to the analysis of KMS states (and KMS functionals) on all of $\mathcal{P}_\Theta$. As announced in the Introduction, here we present some preliminary results that will appear in more detail in a forthcoming publication.

The structure of thermal expectation values can most easily be described by again using (idealized) Fourier transformed, deformed fields $\tilde{\phi}_\theta(p)$ at sharp momenta p; some of the subtleties involved in a mathematically completely rigorous discussion will be mentioned later.

To give a first impression of some of the new aspects that appear, we present the calculation of thermal two-point functions, the simplest non-vanishing n-point functions. Using the symbolic expression $\tilde{\phi}_\theta(p) = \tilde{\phi}(p)U(-\theta p)$ (4) for

the deformed fields, and the exchange relation $U(x)\tilde{\phi}(p) = e^{ip\cdot x}\tilde{\phi}(p)U(x)$ (14) between translation unitaries $U(x)$ and (undeformed) field operators $\tilde{\phi}(p)$, products $\tilde{\phi}_{\theta_1}(p_1)\cdots\tilde{\phi}_{\theta_n}(p_n)$ of deformed fields can be written as products of undeformed fields, multiplied from the right with a translation unitary and a phase factor. Assuming a KMS functional ω on $\mathcal{P}_\Theta$, the task is thus to determine the expectation values of expressions like $\tilde{\phi}(p_1)\cdots\tilde{\phi}(p_n)U(x)$ (where $x = -\sum_{j=1}^n \theta_j p_j$ depends on the θ_j and p_j) in ω. For the case of the two point function, this amounts to determining the expectation value of $\tilde{\phi}(p)\tilde{\phi}(p')U(-\theta p - \theta' p')$ from the KMS condition.

On a formal level, this can be done as follows. Since the translation unitaries $U(x)$ are invariant under the dynamics, we have

$$\tau_t(\tilde{\phi}(p')U(x)) = e^{itp'_0}\tilde{\phi}(p')U(x) \quad \Rightarrow \quad \tau_{t+i\beta}(\tilde{\phi}(p'))U(x) = e^{itp'_0-\beta p'_0}\,\tilde{\phi}(p')U(x)\,. \tag{32}$$

On the other hand, using the exchange relation of $U(x)$ with the Fourier transformed fields, we find

$$\begin{aligned}\tau_t(\tilde{\phi}(p')U(x))\tilde{\phi}(p) &= e^{itp'_0+ix\cdot p}\tilde{\phi}(p')\tilde{\phi}(p)U(x)\\ &= e^{itp'_0+ix\cdot p}\left(\tilde{C}(p',p)U(x) + \tilde{\phi}(p)\tilde{\phi}(p')U(x)\right)\end{aligned} \tag{33}$$

Multiplying (32) from the left with $\tilde{\phi}(p)$ and comparing with (33), we thus see that in a KMS functional ω on $\mathcal{P}_\Theta$, the following equation must hold

$$(e^{-\beta p'_0-ix\cdot p} - 1)\omega(\tilde{\phi}(p)\tilde{\phi}(p')U(x)) = \tilde{C}(p',p)\omega(U(x))\,, \tag{34}$$

and, setting $x = -\theta p - \theta' p'$,

$$\omega(\tilde{\phi}_\theta(p)\tilde{\phi}_{\theta'}(p')) = \omega(U(-\theta p - \theta' p'))\,\frac{\tilde{C}(p,p')}{1 - e^{\beta p^0 + ip\cdot(\theta p + \theta' p')}}\,. \tag{35}$$

This calculation is, of course, only of a formal nature, a rigorous analysis requires in particular a proper treatment of the distributional nature of the appearing fields. Nonetheless, (35) illustrates the main difference to the KMS states on the fiber algebras, where $\theta = \theta'$ is fixed. In that case, the term $\omega(U(x))$ as well as the term $-ix\cdot p$ in the exponential function are not present, because of the translational invariance the commutator $\tilde{C}(p,p')$, leading to $p' = -p$. For $\theta = \theta'$, an analogous calculation directly determines the expressions for (the kernel of) the Fourier-transformed two-point function, up to normalization.

In the case of the full field algebra, however, we retain an expectation value of an element $U(x)$, which is precisely the point already mentioned in the Introduction: Functions of the (vacuum) energy-momentum operators appear in the algebra and their expectation values are a new freedom (not restricted by the KMS condition), which is reflected in the n-point functions.

In other words, $\mathcal{P}_\Theta$ contains a commutative subalgebra $\mathcal{T}_\Theta$ of functions of the momentum operators P, on which the dynamics acts trivially, and we also have to fix ω on this subalgebra. When working with properly smeared fields, $\mathcal{T}_\Theta$ can be identified with certain continuous functions on the joint spectrum of the momentum operators. It then follows that each KMS-*state* ω on $\mathcal{P}_\Theta$ is given by an – a priori arbitrary – *measure* σ (with mass bounded by one) on the energy-momentum spectrum.

By systematically exploiting the KMS condition along the same lines as in the above calculation, the n-point functions can be determined for all $n \in \mathbb{N}$ [26]. These functions (which – by forming linear combinations – also give back the expectation values on $\mathcal{T}_\Theta$), now contain as an additional ingredient the Fourier transform $\tilde{\sigma}$ of the measure σ. More precisely, a modified version $\hat{\sigma}$ of $\tilde{\sigma}$, defined to take the value 1 at the origin but otherwise identical to $\tilde{\sigma}$, appears and is formally related to the expectation values of translation operators by $\omega(U(x)) = \hat{\sigma}(x)$. The n-point functions still have some structural similarity to quasi-free states: they vanish for an odd number of field operators, and for an even number are given by

$$\begin{aligned}&\omega(\tilde{\phi}_{\theta_1}(p_1)\cdots\tilde{\phi}_{\theta_{2n}}(p_{2n}))\\ &\quad= \hat{\sigma}(-\sum_{j=1}^{2n}\theta_j p_j)\prod_{1\le l<r\le 2n} e^{ip_l\cdot\theta_l p_r}\sum_{(\mathbf{l},\mathbf{r})}\prod_{k=1}^{n}\frac{\tilde{C}(p_{l_k},p_{r_k})}{1-e^{\beta p^0_{l_k}+ip_{l_k}\cdot\sum_{b=1}^{2n}\theta_b p_b}},\end{aligned} \tag{36}$$

where the sum runs over all contractions as in (16).

At this point a few remarks are in order.

- Whereas for the undeformed theory, and also for the Moyal-Weyl deformation with fixed θ, the thermal n-point functions for the Klein-Gordon field (with positive mass) are already uniquely determined by the (linear) KMS-condition up to normalization, this condition is much less restrictive for the full field algebra $\mathcal{P}_\Theta$: We have a huge additional freedom when only using the KMS condition; this freedom is parametrized by Fourier transforms of distributions on the energy-momentum spectrum in the vacuum representation. Positivity on $\mathcal{T}_\Theta$ reduces this freedom somewhat, but still all Fourier transforms $\tilde{\sigma}$ of measures on the spectrum remain as possible choices.
- The structures appearing in these calculations look very similar to crossed products from the theory of operator algebras. Furthermore, the calculation of KMS functionals on elements given as undeformed fields times unitaries representing translations can be reinterpreted in terms of a "twisted" KMS condition [5]. We hope to return to these interesting links at a later point.
- The formula (36) should be read as follows: *If* a KMS functional ω exists on $\mathcal{P}_\Theta$, then its n-point functions must have the specified form, with some measure σ. We are currently investigating also the converse direction, namely if given a measure σ on the energy-momentum spectrum, (36) *defines* a (KMS) functional on $\mathcal{P}_\Theta$. To answer this question, one must in particular make sure that the n-point functions (36) yield a well-defined functional ω on $\mathcal{P}_\Theta$. In the case of the

undeformed theory, the algebra $\mathcal{P}_{\{0\}}$ is simple and can be written as a quotient of a free algebra by a (maximal) ideal $\mathcal{J}_{\mathrm{Rel}}$. This ideal is generated by the usual relations (a) linearity of $f \mapsto \phi(f)$, (b) the Klein-Gordon equation, and (c) the commutation relations (13). To formulate a well-defined functional ω on $\mathcal{P}_{\{0\}}$, one therefore only has to check that its n-point functions are consistent with (a)–(c).

In contrast, $\mathcal{P}_\Theta$ is *not* simple. We will consider a non-trivial ideal in it below, but currently have no complete knowledge of its full ideal structure. Nonetheless, we expect that for any measure σ, (36) defines a unique KMS functional on $\mathcal{P}_\Theta$.

We do however not make any claim towards positivity at this stage. Recall that in the case of a single fiber, each normalized KMS functional was automatically positive because of Lemma 2.1(c). This is not the case for the KMS functionals on the full field algebra, and we return to the positivity question below.

- Although the structure of the n-point functions looks similar to the case of single fibers (and thus the non-deformed case), there are now terms involving all momenta instead of only pairs. Furthermore the simple Bose factors are modified by an additional imaginary term in the exponent. These two changes might appear as minor details at first sight, but make it very hard to directly check for positivity (5) of the n-point functions (36). Even simpler, necessary properties of states – like hermiticity, i.e. $\omega(F^*) = \overline{\omega(F)}$ – are not trivial to show.

The main question is now if there are choices for the measure σ such that the above n-point functions determine a *positive* functional, i.e. a state on $\mathcal{P}_\Theta$. To answer this question, it turns out to be most efficient to consider a particular ideal of $\mathcal{P}_\Theta$, instead of directly analyzing the n-point functions.

This ideal is defined as follows: A closer inspection of the subalgebra $\mathcal{T}_\Theta \subset \mathcal{P}_\Theta$ shows that it also contains functions whose support intersects the energy-momentum spectrum only in $\{0\}$, i.e. the one-dimensional projection $E_\Omega = |\Omega\rangle\langle\Omega|$ is an element of $\mathcal{T}_\Theta$. Multiplying this projection from both sides by elements from $\mathcal{P}_\Theta$, one generates an ideal

$$\mathcal{J}_\Theta := \{FE_\Omega G : F, G \in \mathcal{P}_\Theta\} \tag{37}$$

of finite-rank operators, which can be shown to be dense in the C^*-algebra of all compact operators on $\mathcal{H}$.

By standard arguments [4], it follows that any KMS state ω on $\mathcal{P}_\Theta$ must vanish identically on $\mathcal{J}_\Theta$. This implies directly that the measure σ associated with ω must satisfy $\sigma(\{0\}) = 0$. In fact, even more is true: By suitably choosing $F \in \mathcal{P}_\Theta$, one can show that $0 = \omega(FE_\Omega)$ implies that the measure has to vanish altogether, $\sigma = 0$.

Thus all except one of the KMS functionals (36), namely the one given by the zero measure, are *not* positive. In contrast to the undeformed or single fiber case, positivity plays an important role in selecting KMS-states: From an uncountable family of candidate functionals which satisfy the KMS-condition, positivity selects a *unique* one.

Choosing $\sigma = 0$ means that $\hat{\sigma}$ is only non-zero at zero, which leads to a drastic decoupling of the individual fibers: Only n-point functions in which the deformed fields $\phi_{\theta_1}, \ldots, \phi_{\theta_n}$ appear in pairs belonging to the same fiber $\mathcal{P}_{\{\theta_j\}}$ are non-zero. Furthermore, the subalgebra $\mathcal{T}_\Theta$ of functions of momentum operators is mapped to zero except for the case of the identity operator; intuitively the unitaries "average out" by rapid oscillations in the thermodynamic limit.

To show that the remaining KMS functional, associated with the measure $\sigma = 0$, *is* positive, it is best to directly specify its GNS representation, as we shall do next. The GNS space $\mathcal{H}_\Theta$ is a non-separable, infinite tensor product labeled by the elements in the orbit Θ, and the GNS representation π_Θ reads (in the sense of distributions)

$$\pi_\Theta(\tilde{\phi}_\theta(p)) = \big(1 \otimes \cdots \otimes 1 \otimes \pi_0(\tilde{\phi}(p)) \otimes 1 \otimes \cdots \otimes 1\big) \cdot \bigotimes_{\vartheta \in \Theta} U_0(-\vartheta p)\,, \tag{38}$$

where $\pi_0(\tilde{\phi}(p))$ acts on the tensor factor labeled by θ, and π_0 is the GNS representation of the zero fiber w.r.t. its KMS state ω_0. Summing up, we have the following theorem.

Theorem 4.1 *On $\mathcal{P}_\Theta$, for each $\beta > 0$ there exists precisely one KMS state at inverse temperature β. Its n-point functions are* (36) *with $\sigma = 0$, the thermal representation it induces is given by* (38)*.*

From the form of the GNS representation (38), also the mentioned decoupling of the fibers is most transparent: For $\theta \neq \theta'$, one has the exchange relation

$$\pi_\Theta(\tilde{\phi}_\theta(p))\, \pi_\Theta(\tilde{\phi}_{\theta'}(p')) = e^{ip\cdot(\theta+\theta')p'}\, \pi_\Theta(\tilde{\phi}_{\theta'}(p'))\, \pi_\Theta(\tilde{\phi}_\theta(p))\,, \tag{39}$$

and the commutation relation in a fixed fiber are unchanged. This is even stronger than the wedge-local structure mentioned in the Introduction. Whereas in the vacuum representation, $\phi_\theta(f)$ and $\phi_{-\theta}(g)$ commute if the supports of f and g lie in a particular spacelike position depending on θ, in the thermal representation π_Θ we have commutation of $\pi_\Theta(\tilde{\phi}_\theta(f))$ and $\pi_\Theta(\tilde{\phi}_{-\theta}(g))$ for *arbitrary* supports of f, g.

Thus the represented algebra $\pi_\Theta(\mathcal{P}_\Theta)$ appears "more commutative" than its vacuum counterpart $\mathcal{P}_\Theta$, its fibers almost completely decouple at finite temperature. In the context of question (Q3) from the Introduction, this decoupling is the mechanism by which the representation π_Θ becomes wedge-local despite violating the spectrum condition. This however comes at the price of a non-separable representation space, in contrast to the vacuum situation which is better behaved from this point of view. It provides further evidence to the effect that the requirement of a decent thermodynamic behavior can seriously restrict "twist structures", as also observed in supersymmetric theories [5, 6].

Acknowledgements We gratefully acknowledge helpful discussions with D. Buchholz, and the hospitality of the Erwin Schrödinger Institute in Vienna. Initial stages of this work have been supported by the Austrian Science Foundation FWF under the project P22929-N16. GL would also like to thank the organizers of the "Quantum Mathematical Physics" conference for the invitation to Regensburg, where this work was presented.

References

1. H. Araki, J. Woods, Complete Boolean algebras of type I factors. Publ. RIMS, Kyoto University **A2**, 157–242 (1966)
2. A.P. Balachandran, T.R. Govindarajan, Thermofield dynamics and twisted Poincaré symmetry on Moyal space-time. Phys. Rev. **D82**, 105025 (2010)
3. A.P. Balachandran, A. Pinzul, B.A. Qureshi, S. Vaidya, S-Matrix on the Moyal plane: locality versus Lorentz invariance. Phys. Rev. D **77**, 025020 (2008)
4. O. Bratteli, D.W. Robinson, *Operator Algebras and Quantum Statistical Mechanics II* (Springer, Berlin/Heidelberg, 1997)
5. D. Buchholz, R. Longo, Graded KMS functionals and the breakdown of supersymmetry. Adv. Theor. Math. Phys. **3**, 615–626 (1999)
6. D. Buchholz, I. Ojima, Spontaneous collapse of supersymmetry. Nucl. Phys. B **498**(1–2), 228–242 (1997)
7. D. Buchholz, S.J. Summers, *Warped Convolutions: A Novel Tool in the Construction of Quantum Field Theories*, ed. by E. Seiler, K. Sibold. Quantum Field Theory and Beyond: Essays in Honor of Wolfhart Zimmermann (World Scientific, Singapore, 2008), pp. 107–121
8. D. Buchholz, G. Lechner, S.J. Summers, Warped convolutions, Rieffel deformations and the construction of quantum field theories. Commun. Math. Phys. **304**, 95–123 (2011)
9. M. Chaichian, P. Prešnajder, A. Tureanu, New concept of relativistic invariance in NC space-time: twisted Poincaré symmetry and its implications. Phys. Rev. Lett. **94**, 151602 (2005)
10. A.H. Chamseddine, A. Connes, The spectral action principle. Commun. Math. Phys. **186**(3), 731 (1997)
11. A.H. Chamseddine, A. Connes, M. Marcolli, Gravity and the standard model with neutrino mixing. Adv. Theor. Math. Phys. **11**, 991–1089 (2007)
12. A.H. Chamseddine, A. Connes, W.D. van Suijlekom, Inner fluctuations in noncommutative geometry without the first order condition. J. Geom. Phys. **73**, 222–234 (2013)
13. A. Connes, M.R. Douglas, A Schwarz, Noncommutative geometry and matrix theory: compactification on Tori. JHEP **9802**, 003 (1998)
14. A. Devastato, F. Lizzi, P. Martinetti, G. Symmetry, Spectral action, and the Higgs mass. JHEP **1401**, 042 (2014)
15. S. Doplicher, K. Fredenhagen, J.E. Roberts, Space-time quantization induced by classical gravity. Phys. Lett. **B331**, 39–44 (1994)
16. S. Doplicher, K. Fredenhagen, J.E. Roberts, The Quantum structure of space-time at the Planck scale and quantum fields. Commun. Math. Phys. **172**, 187–220 (1995)
17. M.R. Douglas, N.A. Nekrasov, Noncommutative field theory. Rev. Mod. Phys. **73**, 977–1029 (2001)
18. G.G. Emch, *Algebraic Methods in Statistical Mechanics and Quantum Field Theory* (Wiley, New York, 1972)
19. G. Fiore, J. Wess, On 'full' twisted Poincare' symmetry and QFT on Moyal-Weyl spaces. Phys. Rev. **D75**, 105022 (2007)
20. K. Fredenhagen, F. Lindner, Construction of KMS states in perturbative QFT and renormalized Hamiltonian dynamics. Commun. Math. Phys. **332**(3), 895–932 (2014)
21. H. Grosse, G. Lechner, Wedge-local quantum fields and noncommutative Minkowski space. JHEP **11**, 012 (2007)

22. H. Grosse, G. Lechner, Noncommutative deformations of Wightman quantum field theories. JHEP **09**, 131 (2008)
23. H. Grosse, R. Wulkenhaar, The beta-function in duality-covariant noncommutative ϕ^4 theory. Eur. Phys. J. **C35**, 277–282 (2004)
24. H. Grosse, R. Wulkenhaar, Renormalisation of ϕ^4 theory on noncommutative R^4 in the matrix base. Commun. Math. Phys. **256**, 305–374 (2005)
25. R. Haag, N.M. Hugenholtz, M. Winnink, On the equilibrium states in quantum statistical mechanics. Commun. Math. Phys. **5**, 215–236 (1967)
26. A. Huber, Thermal equilibrium states in deformed quantum field theory. Master's thesis, University of Vienna, 2012
27. D. Kaschek, N. Neumaier, S. Waldmann, Complete positivity of Rieffel's deformation quantization by actions of R^d. J. Noncommutative Geom. **3**, 361–375 (2009)
28. A. Lakhoua, F. Vignes-Tourneret, J.-C. Wallet, One-loop beta functions for the orientable non-commutative Gross–Neveu model. Eur. Phys. J. C **52**(3), 735 (2007)
29. G. Lechner, Deformations of quantum field theories and integrable models. Commun. Math. Phys. **312**(1), 265–302 (2012)
30. E. Morfa-Morales, Deformations of quantum field theories on curved spacetimes. Ph.D. thesis, University of Vienna, 2012
31. G. Piacitelli, Twisted covariance as a non invariant restriction of the fully covariant DFR model. Commun. Math. Phys. **295**, 701–729 (2010)
32. M.A. Rieffel, *Deformation Quantization for Actions of* R^d. Memoirs of the Amerian Mathematical Society, vol. 106 (American Mathematical Society, Providence, 1992)
33. V. Rivasseau, Non-commutative renormalization. Séminaire Poincaré X, 2007, pp. 15–95
34. N. Seiberg, E. Witten, String theory and noncommutative geometry. JHEP **09**, 032 (1999)
35. M.A. Soloviev, On the failure of microcausality in noncommutative field theories. Phys. Rev. **D77**, 125013 (2008)
36. H. Steinacker, Emergent gravity from noncommutative gauge theory. JHEP **0712**, 049 (2007)
37. R.F. Streater, A. Wightman, *PCT, Spin and Statistics, and All That* (Benjamin-Cummings, Reading, 1964)
38. S.J. Summers, A perspective on constructive quantum field theory (2012, Preprint). arXiv:1203.3991
39. J. Zahn, Remarks on twisted noncommutative quantum field theory. Phys. Rev. **D73**, 105005 (2006)

Kinematical Foundations of Loop Quantum Cosmology

Christian Fleischhack

Contents

C. Fleischhack (✉)
Institut für Mathematik, Universität Paderborn, 33095 Paderborn, Germany
e-mail: fleischh@math.upb.de

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_11

Abstract First, we review the C^*-algebraic foundations of loop quantization, in particular, the construction of quantum configuration spaces and the implementation of symmetries. Then, we apply these results to loop quantum gravity, focusing on the space of generalized connections and on measures thereon. Finally, we study the realm of homogeneous isotropic loop quantum cosmology: once viewed as the loop quantization of classical cosmology, once seen as the symmetric sector of loop quantum gravity. It will turn out that both theories differ, i.e., quantization and symmetry reduction do not commute. Moreover, we will present a uniqueness result for kinematical measures. These last two key results have originally been due to Hanusch; here, we give drastically simplified and direct proofs.

Keywords Loop quantization • Gravity • Cosmology • Abelian C^* algebras • Quantum symmetries • Invariant connections

Mathematics Subject Classification (2010). Primary 46L60; Secondary 58D19, 46L65, 81T05, 83C45, 83F05

1 Introduction

The quantization of gravity is one of the grand unsolved problems in mathematical physics. As can be seen from this edited volume again, there are several different attempts to disclose at least glimpses of the desired theory. Loop quantum gravity [9, 53], the approach that sets the framework for the present contribution, is one of them. It originates in a formulation of gravity, by means of so-called Ashtekar variables [2], as a canonical gauge field theory with constraints that is quantized along the ideas of Dirac [5, 10]. The kinematical part of loop quantum gravity has been well understood; there are even very strong uniqueness results [29, 44] that play the same role as the Stone-von Neumann theorem for quantum mechanics. However, despite the marvelous results obtained by Thiemann et al. [53] and references therein, our knowledge about dynamical consequences of the theory is still rather poor. What to do?

One strategy to investigate complicated physical theories is to study toy models with special symmetries hoping that these models exhibit key features of the full system. In particular, gravity has very much profited from such ideas. Among the first solutions to Einstein's equations, there have been the Schwarzschild solution corresponding to spherically symmetric black holes or the Friedmann solutions that describe homogeneous and isotropic universes. All these have been results within classical gravity. But also in loop quantum gravity, the reduce-symmetry strategy has been successfully implemented. Some 15 years ago, Bojowald, based on his idea with Kastrup [20], invented a theory, now called loop quantum cosmology [11]. He simply quantized cosmological models along the lines of the full theory. It brought about many interesting results like the resolution of big-bang singularities [18] or

later big-bounce scenarios [12]. As one had hoped, the dynamics of loop quantum cosmology was much easier accessible, indeed.

The relation between loop quantum gravity and loop quantum cosmology, however, has remained unclear. Before explaining this, let us recall some key ingredients of the loop approach [5, 6, 10, 23]. First, there is some quantum configuration space $\overline{\mathcal{X}}$, which is compact and contains the classical one as a dense subset. Second, $\overline{\mathcal{X}}$ admits some appropriate measure μ that induces the kinematical L^2 Hilbert space. Finally, states are constructed using Gelfand triples. Now, the original idea of Bojowald and Kastrup [20] was as follows: consider the cosmological configuration space as a subset of that of full gravity, and continuously extend this embedding to the corresponding quantum configuration spaces. Based on this extension, one constructs the algebras of basic variables and finally the states by duality.

This connection, however, broke down when Brunnemann and the author [21] discovered that there is *no* continuous extension of the embedding at classical level to one at quantum level. Note that this does not mean that loop quantum gravity or loop quantum cosmology considered as theories of their own are now wrong; it has merely been the bridge between both theories that has been destroyed.

In order to fill that conceptual gap, the kinematics of loop quantum cosmology has had to be carefully revisited. In the present article, we would like to report on the present status of this endeavor [23, 31, 38]. For this, we will first outline the mathematical theory of how to construct quantum configuration spaces in the loop quantization framework, then apply it to loop quantum gravity and finally discuss all the (kinematical) issues above for homogeneous isotropic cosmologies, being in some sense the easiest example. It will surprisingly turn out that the original idea of Bojowald-Kastrup remains valid if one modifies their quantum configuration space appropriately.

2 Quantization and Symmetries

The configuration space of loop quantum gravity has originally been obtained using C^*-algebras [5]. Later, it has been shown that it can also be identified with a certain projective limit [7, 8]. Although the latter framework is better suited for the construction of measures, the C^*-algebraic approach has turned out best suited for our purposes, namely quantization *and* implementation of symmetries. Its basic idea is as follows: One starts with an arbitrary classical configuration space $\mathcal{X}$. Then, one chooses some C^*-algebra $\mathfrak{A}$ consisting of bounded complex-valued functions on $\mathcal{X}$ that are to be quantized in some sense; this is the core part of loop quantization. To implement symmetries, as usual, one assumes to be given a symmetry group S acting[1] on $\mathcal{X}$. This allows to perform

[1] One may assume w.l.o.g. that the action is effective although we will never use this.

- **Quantization**
  The quantum configuration space $\overline{\mathcal{X}}$ is simply the spectrum of $\mathfrak{A}$.
- **Symmetry Reduction**
  The classical reduced configuration space $\mathcal{X}_{\text{red}}$ comprises the elements in $\mathcal{X}$ that are invariant w.r.t. the symmetry group S.

One is now immediately tempted to ask:

- **Quantization ∘ Symmetry Reduction**
  Can we quantize the reduced classical configuration space as the full one? And how are the quantum configuration spaces of the full theory and the reduced theory related? – Well, it will turn out, that the answer crucially depends on the choice of the algebra in the symmetric case.
- **Symmetry Reduction ∘ Quantization**
  Can we implement symmetries even on quantum level? – Yes, provided the underlying algebra is invariant.

This leads us to the most important question: Does it matter whether we implement symmetry *before* or *after* quantization? Or even shorter:

Do quantization and symmetry reduction commute?

Unfortunately, there is no general answer. But at least for some particular cases in loop quantum cosmology, the answer is known as we will have learned by the end of this review.

To start with the general framework, in Sect. 2.1, we review the definition of quantum configuration spaces from [23].[2] Then, in Sect. 2.2 we review, again from [23], a criterion guaranteeing that a mapping between classical configuration spaces can be lifted to their quantum counterparts. The lifting is functorial (Sect. 2.3), which allows to lift even group actions (Sect. 2.4). Finally, in Sect. 2.5, we review the results from [38] on the relations between the quantum symmetric and the symmetric quantum configuration spaces.

2.1 Quantum Configuration Spaces

Recall [46] that the spectrum of an abelian C^*-algebra $\mathfrak{A}$ consists of all nontrivial multiplicative linear functionals on $\mathfrak{A}$. The Gelfand transform $\tilde{a}$ of any $a \in \mathfrak{A}$ is given by

$$\begin{aligned} \tilde{a} : \operatorname{spec}\mathfrak{A} &\longrightarrow \mathbb{C}\,. \\ \chi &\longmapsto \chi(a) \end{aligned}$$

[2] Parts of Proposition 1 originate in [47].

The topology on spec $\mathfrak{A}$ is the initial topology induced by all the Gelfand transforms. The celebrated Gelfand-Naimark theorem states that $a \longmapsto \tilde{a}$ is an isometric $*$-isomorphism between $\mathfrak{A}$ and $C_0(\text{spec}\,\mathfrak{A})$. If now $\mathfrak{A}$ is an algebra of functions on some configuration space $\mathcal{X}$, then the evaluation mapping provides us with a natural embedding of $\mathcal{X}$ into spec $\mathfrak{A}$.

Proposition 1 *Let $\mathcal{X}$ be a set and $\mathfrak{A} \subseteq \ell^\infty(\mathcal{X})$ a C^*-subalgebra with empty kernel.*[3] *Then the* ***natural mapping*** $\iota : \mathcal{X} \longrightarrow \text{spec}\,\mathfrak{A}$ *defined by the evaluation mapping*

$$\begin{aligned} \iota(x) : \mathfrak{A} &\longrightarrow \mathbb{C} \\ a &\longmapsto a(x) \end{aligned}$$

is well defined and has the following properties:

1. $\tilde{a} \circ \iota = a$ *for all* $a \in \mathfrak{A}$.
2. $\iota(\mathcal{X})$ *is dense in* spec $\mathfrak{A}$.
3. ι *and* $\mathfrak{A}$ *separate the same points.*
4. ι *is injective* $\Longleftrightarrow$ $\mathfrak{A}$ *separates the points in* $\mathcal{X}$.
5. ι *is continuous* $\Longleftrightarrow$ $\mathfrak{A}$ *consists of continuous functions on* $\mathcal{X}$ *only.*

Here, for the final assertion, we assumed $\mathcal{X}$ to be given some topology.

Proof Well-definedness follows from the empty-kernel assumption.

1. Observe $[\tilde{a} \circ \iota](x) \equiv \tilde{a}(\iota(x)) = [\iota(x)](a) = a(x)$.
2. Let $\chi \in \text{spec}\,\mathfrak{A}$ be outside the closure of $\iota(\mathcal{X})$. Then, by regularity of locally compact Hausdorff spaces, there is some $\phi = \tilde{a} \in C_0(\text{spec}\,\mathfrak{A})$ with $\phi(\chi) \neq 0$, but $\phi \equiv 0$ on $\iota(\mathcal{X})$. This implies $a = \tilde{a} \circ \iota = \phi \circ \iota = 0$ and $\phi \equiv 0$.
3. Observe $\iota(x) = \iota(x') \Longleftrightarrow a(x) \equiv \iota(x)(a) = \iota(x')(a) \equiv a(x')$ for all $a \in \mathfrak{A}$.
4. This follows immediately from the previous item.
5. By definition of the Gelfand-Naimark topology, ι is continuous iff $a \equiv \tilde{a} \circ \iota : \mathcal{X} \longrightarrow \mathbb{C}$ is continuous for all a. □

Definition 2 The **quantum configuration space** $\overline{\mathcal{X}}$ is the spectrum of $\mathfrak{A}$.

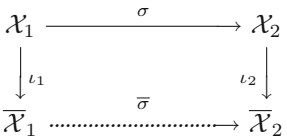
We will refer to $\mathfrak{A}$ as the corresponding **quantizing algebra**. This algebra should be rich enough to separate the points of $\mathcal{X}$ and to contain sufficiently many physically "interesting" functions. Note, however, that the definition of $\overline{\mathcal{X}}$ crucially depends on the choice of $\mathfrak{A}$. This will become relevant in loop quantum cosmology.

[3] The kernel of $\mathfrak{A}$ is defined by $\bigcap_{a \in \mathfrak{A}} a^{-1}(0)$. In particular, each unital $\mathfrak{A}$ has empty kernel. Throughout the whole article, any $\mathfrak{A}$ will have empty kernel – or we will assume that.

2.2 *Lifting Criteria*

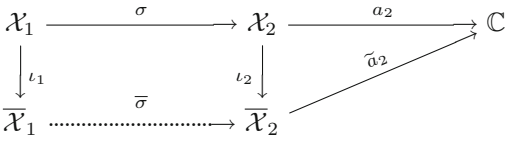
In the next step, we are going to compare different quantum configuration spaces. More concretely, we assume to be given two classical configuration spaces $\mathcal{X}_1$ and $\mathcal{X}_2$ that are related by some mapping $\sigma : \mathcal{X}_1 \longrightarrow \mathcal{X}_2$. There are two prime examples we will be interested in: First, $\mathcal{X}_1$ is a subset of $\mathcal{X}_2$, given by certain invariant elements in $\mathcal{X}_2$, with σ being the canonical embedding; second, both spaces coincide and σ is some isomorphism, e.g., obtained from some group action. How can we relate the corresponding quantum configuration spaces? A very natural notion is obviously that of a lift[4]:

Definition 3 $\overline{\sigma}$ is a **lift** of σ (w.r.t. some algebras $\mathfrak{A}_1$ and $\mathfrak{A}_2$) iff it fills the diagram



Is there always a lift $\overline{\sigma} : \overline{\mathcal{X}}_1 \longrightarrow \overline{\mathcal{X}}_2$ filling this diagram? Under which circumstances is $\overline{\sigma}$ unique? When is it continuous? When injective?

To get an idea how to answer these questions, assume that such a continuous lift $\overline{\sigma}$ exists for unital $\mathfrak{A}_1$. Then, for any $a_2 \in \mathfrak{A}_2$, the function $\tilde{a}_2 \circ \overline{\sigma} : \overline{\mathcal{X}}_1 \longrightarrow \mathbb{C}$ is continuous, hence equals $\tilde{a}_1$ for some $a_1 \in \mathfrak{A}_1$ by Gelfand-Naimark (and unitality of $\mathfrak{A}_1$). Moreover,



commutes, and we have

$$\sigma^* a_2 \;\equiv\; a_2 \circ \sigma \;=\; \tilde{a}_2 \circ \overline{\sigma} \circ \iota_1 \;=\; \tilde{a}_1 \circ \iota_1 \;=\; a_1 \;\in\; \mathfrak{A}_1 \,.$$

[4] If the natural mappings ι_i are injective, this just means that $\overline{\sigma}$ extends σ.

This motivates to define the **restriction algebra**[5] of $\mathfrak{A}_2$ w.r.t. σ by

$$\sigma^*\mathfrak{A}_2 \;:=\; \{\sigma^* a_2 \mid a_2 \in \mathfrak{A}_2\} \;\subseteq\; \ell^\infty(\mathcal{X}_1)\,.$$

Thus, we have shown that $\sigma^*\mathfrak{A}_2 \subseteq \mathfrak{A}_1$ is necessary for the existence of $\overline{\sigma}$. But, could this condition even be sufficient as well?

So, let us assume $\sigma^*\mathfrak{A}_2 \subseteq \mathfrak{A}_1$. Then, by Proposition 1_3, we have

$$\begin{aligned} \iota_1(x_1) = \iota_1(x_1') &\iff a_1(x_1) = a_1(x_1') \quad \forall\ a_1 \\ &\implies a_2(\sigma(x_1)) = a_2(\sigma(x_1')) \quad \forall\ a_2 \\ &\iff \iota_2(\sigma(x_1)) = \iota_2(\sigma(x_1')) \end{aligned}$$

whence $\widehat{\sigma} := \iota_2 \circ \sigma \circ \iota_1^{-1} : \iota_1(\mathcal{X}_1) \longrightarrow \overline{\mathcal{X}}_2$ is well defined. Moreover, we have

$$(\sigma^* a_2)^\sim \circ \iota_1 \;=\; \sigma^* a_2 \;=\; \tilde{a}_2 \circ \iota_2 \circ \sigma \;=\; \tilde{a}_2 \circ \widehat{\sigma} \circ \iota_1$$

for any $a_2 \in \mathfrak{A}_2$. In particular, $(\sigma^* a_2)^\sim$ is a continuous continuation of $\tilde{a}_2 \circ \widehat{\sigma}$ on $\overline{\mathcal{X}}_1$. As $\iota_1(\mathcal{X}_1)$ is dense in the compact space $\overline{\mathcal{X}}_1$, one shows quickly that $\widehat{\sigma}$ can be extended to a continuous mapping $\overline{\sigma}$ on $\overline{\mathcal{X}}_1$. In particular, it fulfills

$$(\sigma^* a_2)^\sim \;=\; \tilde{a}_2 \circ \overline{\sigma} \tag{1}$$

for all $a_2 \in \mathfrak{A}_2$. Altogether, we have derived

Proposition 4 *For unital $\mathfrak{A}_1$, there is a continuous lift of σ iff $\sigma^*\mathfrak{A}_2 \subseteq \mathfrak{A}_1$.*

Uniqueness of $\overline{\sigma}$ is obvious as $\iota_1(\mathcal{X}_1)$ is always dense. So, given existence, it remains to find a criterion for injectivity of $\overline{\sigma}$. For this, observe first that we obtain from (1) and Proposition 1_1

$$\bar{x}_1(\sigma^* a_2) \;=\; (\sigma^* a_2)^\sim(\bar{x}_1) \;=\; [\tilde{a}_2 \circ \overline{\sigma}](\bar{x}_1) \;=\; [\overline{\sigma}(\bar{x}_1)](a_2)$$

for any $\bar{x}_1 \in \overline{\mathcal{X}}_1$ and $a_2 \in \mathfrak{A}_2$, hence

Lemma 5 *If $\mathfrak{A}_1$ is unital and $\overline{\sigma}$ exists, then for all $\bar{x}_1 \in \overline{\mathcal{X}}_1$*

$$\overline{\sigma}(\bar{x}_1) = \bar{x}_1 \circ \sigma^*\,.$$

[5] To explain the term "restriction algebra", assume that σ is injective, whence $\mathcal{X}_1$ can be considered as a subset of $\mathcal{X}_2$. Then $\sigma^*\mathfrak{A}_2$ consists just of the restrictions of the functions in $\mathfrak{A}_2 \subseteq \ell^\infty(\mathcal{X}_2)$ to the domain $\mathcal{X}_1$. In order to avoid conflicts with the different notion of pull-back C^*-algebras, we will use the notion "restriction algebra" also in the case where σ is not injective.

This now implies

$$\overline{\sigma}(\overline{x}_1) = \overline{\sigma}(\overline{x}'_1) \Longleftrightarrow \overline{x}_1(\sigma^* a_2) = \overline{x}'_1(\sigma^* a_2) \quad \forall\, a_2 \in \mathfrak{A}_2\,.$$

Consequently, $\overline{\sigma}$ is injective iff $\overline{\mathcal{X}}_1 = \operatorname{spec} \mathfrak{A}_1$ separates to points in $\sigma^*\mathfrak{A}_2 \subseteq \mathfrak{A}_1$, which is equivalent to the denseness of $\sigma^*\mathfrak{A}_2$ in $\mathfrak{A}_1$ by the Stone-Weierstraß and the Gelfand-Naimark theorems, provided $\sigma^*\mathfrak{A}_2$ is unital. Altogether, we have

Theorem 6 *Let $\mathfrak{A}_1$ and $\mathfrak{A}_2$ be unital. Then*

$$\sigma : \mathcal{X}_1 \longrightarrow \mathcal{X}_2 \textit{ has a continuous injective lift} \Longleftrightarrow \sigma^*\mathfrak{A}_2 \textit{ is dense in } \mathfrak{A}_1$$

Moreover, the lift is unique if existing.

Note that we did *not* require σ to fulfill any continuity condition. Indeed, we get the continuity of $\overline{\sigma}$ for free from the C^*-algebra construction.

For practical purposes, it is often nicer to use the criterion

Corollary 7 *Let $\mathfrak{A}_1$ and $\mathfrak{A}_2$ be unital, and let $\mathfrak{B}_2$ be a dense $*$-algebra in $\mathfrak{A}_2$. Then we have*

$$\sigma : \mathcal{X}_1 \longrightarrow \mathcal{X}_2 \textit{ has a continuous injective lift} \Longleftrightarrow \sigma^*\mathfrak{B}_2 \textit{ is dense in } \mathfrak{A}_1$$

Proof Observe that $\overline{\sigma^*\mathfrak{B}_2}$ always equals $\overline{\sigma^*\mathfrak{A}_2}$, since

$$\sigma^*\mathfrak{B}_2 \;\subseteq\; \sigma^*\mathfrak{A}_2 \;\equiv\; \sigma^*\overline{\mathfrak{B}_2} \;\subseteq\; \overline{\sigma^*\mathfrak{B}_2}.$$

Now the statement follows from Theorem 6 immediately. □

These criteria directly suggest what to do if one wants to embed the quantum configuration space for $\mathcal{X}_1$ into that of $\mathcal{X}_2$, given some σ. Simply *define* the algebra $\mathfrak{A}_1$ to be the completion of $\sigma^*\mathfrak{A}_2$. We will apply this strategy to the case of loop quantum cosmology in Sect. 4, where $\mathcal{X}_2$ is the configuration space of full gravity and $\mathcal{X}_1$ that of symmetric configurations describing a certain cosmology. But, before that, we shall discuss how to lift group actions from any classical configuration space to its quantum counterpart.

2.3 Functoriality

Having seen how to lift configuration spaces from the classical to the quantum level, but also how to lift mappings between them, it is very natural to ask whether these

constructions are in some sense functorial. Indeed, they are. Consider the diagram:

$$\begin{array}{ccccc} \mathcal{X}_1 & \xrightarrow{\quad\sigma\quad} & \mathcal{X}_2 & \xrightarrow{\quad\tau\quad} & \mathcal{X}_3 \\ \downarrow{\scriptstyle \iota_1} & & \downarrow{\scriptstyle \iota_2} & & \downarrow{\scriptstyle \iota_3} \\ \overline{\mathcal{X}}_1 & \xrightarrow{\quad\overline{\sigma}\quad} & \overline{\mathcal{X}}_2 & \xrightarrow{\quad\overline{\tau}\quad} & \overline{\mathcal{X}}_3 \end{array}$$

Here, our lifting criterion tells us that $\overline{\sigma}$ exists iff $\sigma^*\mathfrak{A}_2 \subseteq \mathfrak{A}_1$ and that $\overline{\tau}$ exists iff $\tau^*\mathfrak{A}_3 \subseteq \mathfrak{A}_2$. Together, we see that the liftability of σ and τ implies that

$$(\tau \circ \sigma)^*\mathfrak{A}_3 \;\equiv\; \sigma^*(\tau^*\mathfrak{A}_3) \;\subseteq\; \sigma^*\mathfrak{A}_2 \;\subseteq\; \mathfrak{A}_1,$$

i.e., $\tau \circ \sigma$ is liftable as well. From the uniqueness part, we get immediately

$$\overline{\tau \circ \sigma} = \overline{\tau} \circ \overline{\sigma}\,.$$

Finally, even the embedding criterion is functorial. Indeed, assume that σ and τ lift to embeddings, i.e., $\sigma^*\mathfrak{A}_2$ is dense in $\mathfrak{A}_1$ as well as $\tau^*\mathfrak{A}_3$ is dense in $\mathfrak{A}_2$. Now,

$$\sigma^*\mathfrak{A}_2 \;=\; \sigma^*(\overline{\tau^*\mathfrak{A}_3}) \;\subseteq\; \overline{\sigma^*(\tau^*\mathfrak{A}_3)} \;=\; \overline{(\tau \circ \sigma)^*\mathfrak{A}_3} \;\subseteq\; \overline{\mathfrak{A}_1} \;\equiv\; \mathfrak{A}_1$$

implies that $(\tau \circ \sigma)^*\mathfrak{A}_3$ is dense in $\mathfrak{A}_1$.

2.4 Group Actions

This functoriality immediately allows us to lift group actions. For this, let $\mathcal{X}$ be some set and $\mathfrak{A}$ be again some C^*-subalgebra of $\ell^\infty(\mathcal{X})$. Recall that a (left) action of a group S on $\mathcal{X}$ consists of mappings $\varphi_s : \mathcal{X} \longrightarrow \mathcal{X}$ that fulfill $\varphi_{\mathbf{1}} = \mathrm{id}$ as well as $\varphi_{s_1 s_2} = \varphi_{s_1} \circ \varphi_{s_2}$ for all $s_1, s_2 \in S$. Ignoring continuity or smoothness issues for the moment, we see that φ_s can be lifted to the quantum level iff $\varphi_s^*\mathfrak{A} \subseteq \mathfrak{A}$. In order to lift all φ_s, we just have to require that $\mathfrak{A}$ is S-invariant, i.e., $\varphi_s^*\mathfrak{A} = \mathfrak{A}$ for all $s \in S$. Moreover, functoriality shows that $\overline{\varphi_{s_1 s_2}} = \overline{\varphi_{s_1}} \circ \overline{\varphi_{s_2}}$. As obviously the identity is lifted to the identity, we even see that each $\overline{\varphi_s}$ is a homeomorphism on $\overline{\mathcal{X}}$ with $\overline{\varphi_s}^{-1} = \overline{\varphi_{s^{-1}}}$. Altogether, we have

Theorem 8 *A group action on $\mathcal{X}$ lifts to a group action on $\overline{\mathcal{X}}$ iff $\mathfrak{A}$ is S-invariant. The lifted group action is even unique, and each group element acts by homeomorphisms on $\overline{\mathcal{X}}$ fulfilling*

$$\overline{\varphi}_s(\overline{x}) = \overline{x} \circ \varphi_s^* \tag{2}$$

with $\overline{\varphi}$ denoting the lifted action of S on $\overline{\mathcal{X}}$ defined by $\overline{\varphi}_s := \overline{\varphi_s}$.

The issue of continuity is a bit more subtle. For topological groups S, one can show [38, 39] by methods from C^*-dynamical systems that $\overline{\varphi} : S \times \overline{\mathcal{X}} \longrightarrow \overline{\mathcal{X}}$ is continuous if $s \longmapsto a \circ \varphi_s$ is continuous for all $a \in \mathfrak{A}$; the converse is true if $\mathfrak{A}$ is unital. Remarkably, this is completely independent from whether φ is continuous or not. Indeed, in the relevant cases of loop quantum cosmology or loop quantum gravity the action on the classical level is not necessarily smooth. But even in these cases, we already get for free that $\overline{\varphi}_s$ is always a homeomorphism.

2.5 Symmetric Sectors

The presence of a group action immediately leads us to the notion of invariant (or symmetric) elements. Here, the situation is even more interesting: we have group actions both on the classical and on the quantum level. Can we relate both levels?

To be more specific, first define the symmetric classical set by

$$\mathcal{X}_{\mathrm{red}} := \{x \in \mathcal{X} \mid \varphi_s(x) = x \quad \forall\, s \in S\}$$

and, analogously, the symmetric quantum space by

$$\overline{\mathcal{X}}_{\mathrm{red}} := \{\bar{x} \in \overline{\mathcal{X}} \mid \overline{\varphi}_s(\bar{x}) = \bar{x} \quad \forall\, s \in S\}\,.$$

At the same time, however, we can consider the space $\mathcal{X}_{\mathrm{red}}$ of symmetric classical configurations as a configuration space in its own right. This has been precisely the standard way of thinking in loop quantum cosmology. In particular, we can quantize it given some reasonable abelian C^*-algebra $\mathfrak{A}_{\mathrm{red}}$ of bounded functions on it. This algebra can, in principle, be chosen quite arbitrarily. If, however, one wants to embed the quantized reduced space $\overline{\mathcal{X}_{\mathrm{red}}}$ into the quantized full space $\overline{\mathcal{X}}$, one has to define $\mathfrak{A}_{\mathrm{red}}$ by $\overline{\mathfrak{A}|_{\mathcal{X}_{\mathrm{red}}}}$. It is now natural to ask how the spaces $\overline{\mathcal{X}}_{\mathrm{red}}$ and $\overline{\mathcal{X}_{\mathrm{red}}}$ as well as the closure of $\iota(\mathcal{X}_{\mathrm{red}})$ in $\overline{\mathcal{X}}$ are related. Here, $\mathcal{X}_{\mathrm{red}}$ is considered as a subset of $\mathcal{X}$.

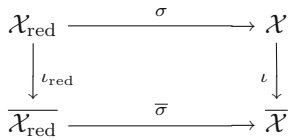
Theorem 9 *We have*

1. $\overline{\mathcal{X}_{\mathrm{red}}}$ *is homeomorphic to* $\overline{\iota(\mathcal{X}_{\mathrm{red}})}$*, provided* $\mathfrak{A}$ *is unital.*
2. $\overline{\iota(\mathcal{X}_{\mathrm{red}})}$ *is contained in* $\overline{\mathcal{X}}_{\mathrm{red}}$.
3. $\overline{\mathcal{X}}_{\mathrm{red}}$ *is closed in* $\overline{\mathcal{X}}$.

Note that later we will identify $\overline{\mathcal{X}_{\mathrm{red}}}$ and $\overline{\iota(\mathcal{X}_{\mathrm{red}})}$.

Proof

1. Let $\sigma : \mathcal{X}_{\rm red} \longrightarrow \mathcal{X}$ be the inclusion mapping[6] and let $\overline{\sigma}$ be the corresponding lift:



   Now, $\overline{\sigma} \circ \iota_{\rm red} = \iota \circ \sigma$ and the continuity of $\overline{\sigma}$ give

$$\begin{aligned} \iota(\sigma(\mathcal{X}_{\rm red})) &\equiv \overline{\sigma}(\iota_{\rm red}(\mathcal{X}_{\rm red})) \\ &\subseteq \overline{\sigma}(\overline{\iota_{\rm red}(\mathcal{X}_{\rm red})}) \;\subseteq\; \overline{\overline{\sigma}(\iota_{\rm red}(\mathcal{X}_{\rm red}))} \;\equiv\; \overline{\iota(\sigma(\mathcal{X}_{\rm red}))}\,, \end{aligned}$$

   hence, by compactness of $\overline{\iota_{\rm red}(\mathcal{X}_{\rm red})}$,

$$\overline{\iota(\mathcal{X}_{\rm red})} \;\equiv\; \overline{\iota(\sigma(\mathcal{X}_{\rm red}))} = \overline{\sigma}(\overline{\iota_{\rm red}(\mathcal{X}_{\rm red})}) \;\equiv\; \overline{\sigma}(\overline{\mathcal{X}_{\rm red}})\,.$$

   Now, the proof follows as $\overline{\sigma}$, by unitality, maps a compact space into a Hausdorff space, hence is a homeomorphism onto its image.
2. Since $\overline{\varphi}_s \circ \iota = \iota \circ \varphi_s$, each element of $\iota(\mathcal{X}_{\rm red})$ is invariant under each $\overline{\varphi}_s$.
3. If the net $(\overline{x}_\alpha) \subseteq \overline{\mathcal{X}}$ converges to $\overline{x} \in \overline{\mathcal{X}}$, then $\overline{\varphi}_s(\overline{x}_\alpha) \to \overline{\varphi}_s(\overline{x})$ by continuity of $\overline{\varphi}_s$. Closedness of $\overline{\mathcal{X}}_{\rm red}$ is now obvious.

□

It now remains to decide whether the inclusion relation between $\overline{\mathcal{X}_{\rm red}}$ and $\overline{\mathcal{X}}_{\rm red}$ is proper. More literally: can any invariant quantum configuration be approximated by invariant classical configurations? Seen functorially on the level of configuration spaces, this means: do quantization and symmetry implementation commute?

The general answer is – well, it depends. Indeed, we are neither aware of nor have we been able to so far find general conditions that imply commutativity – or non-commutativity. In loop quantum cosmology, however, the usual answer is negative: quantization and reduction do not commute. We will discuss this issue in Sect. 4.8.

3 Loop Quantum Gravity

Having settled the general mathematical framework for the quantization scheme used in loop quantization, we are now going to apply it to gravity. First, in Sect. 3.1, we review the classical configuration space of general relativity, both for

[6] Note that later we will refrain from writing σ in the case of subspaces of invariant elements.

metric and for Ashtekar variables. Then, following [8, 24], we describe its loop quantum counterpart in three equivalent forms: as the spectrum of a C^*-algebra, as homomorphisms of the path groupoid and as a projective limit of Lie groups. The Ashtekar-Lewandowski measure [6] is described in Sect. 3.5, before we conclude with an explicit example [24] of an element of the quantum configuration space and with the discussion of the underlying smoothness category.

3.1 Classical Configuration Space

As we have learned in Sect. 2, we need two pieces of information to define the quantum configuration space of a physical theory: the classical configuration space $\mathcal{X}$ and some algebra $\mathfrak{A}$ of bounded functions thereon. Let us start with the classical configuration space, now for gravity.

Metric Variables

Classical gravity, or general relativity, is described by a spacetime metric g fulfilling the Einstein equations $G + \Lambda g = 8\pi T$. Here, a spacetime metric is a metric of Lorentzian signature on a 4-dimensional, connected, time-oriented and oriented manifold. Moreover, the Einstein tensor G is defined by $G := R - \frac{1}{2}R_{\mathrm{scal}}g$, with R and R_{scal} being the Ricci and the scalar curvatures of g, respectively. Finally, Λ is the cosmological constant and T is the stress-energy tensor. We will set both terms to zero, this way restricting ourselves to matter-free gravity in the vacuum.

Conceptually, general relativity is a covariant theory. Technically, it requires to solve a nonlinear partial differential equation. At the same time, it is desirable to formulate general relativity as an initial value problem, i.e. as a canonical theory. However, canonical theories require some distinguished time variable, not naturally given in relativistic theories. Nevertheless, there is a class of spacetimes that admit a well-posed initial value formulation, namely globally hyperbolic spacetimes [54]. Originally, this notion had referred to the causal structure of the spacetime metric. According to the celebrated results by Bernal and Sánchez [16, 17], it is equivalent to the assumption that the spacetime manifold M is diffeomorphic to $\mathbb{R} \times \Sigma$ for some 3-manifold Σ and that the Lorentzian metric is given by $-f_\tau \, \mathrm{d}\tau^2 + q_\tau$ for some smooth families f_τ and q_τ of functions and Riemannian metrics on Σ, respectively. Moreover, each level set $\Sigma_\tau := \{\tau\} \times \Sigma$ is then a Cauchy surface; usually, one simply identifies Σ with Σ_0.

Now, given global hyperbolicity, we can consider Einstein's equations as an initial-value problem. For this, one first observes that any spacetime metric on M can be uniquely reconstructed from its restriction q to Σ_τ and from the second fundamental form (or, extrinsic curvature) K describing the shape of Σ_τ as a

submanifold of M. Einstein's equations transfer to some evolution equations for q and K, but also imply that these two objects have to fulfill certain constraint equations, namely the diffeomorphism constraint and the Hamilton constraint. They encode the invariance of the theory under spatial and temporal diffeomorphisms. It is a very remarkable result that our initial-value problem can now be solved at least locally [34, 48, 50] iff these constraints are met. One can even show that the metric q on Σ and some expression being linear (up to some weight) in K are canonically conjugate variables. Thus, we can consider the space of Riemannian 3-metrics on Σ as the (unconstrained) configuration space of canonical general relativity.[7]

Ashtekar Variables

The configuration space of Riemannian metrics became the starting point of the Wheeler-DeWitt approach to quantum gravity. Its idea was basically to consider quantum gravity as quantum mechanics of metrics, with the Hamilton constraint inducing the Hamiltonian. Technically, the non-polynomiality of the Hamilton constraint, however, was a big issue. In the 1980s, Ashtekar [2, 3] tried to cure that problem introducing new variables, now carrying his name.

First, he encoded the metric by means of triads. Of course, each triad determines a metric by requiring it to be oriented orthonormal. However, the other direction is not unique. In fact, each metric admits a whole bunch of oriented orthonormal triads; more precisely, two triads give the same metric iff they are related by some $SO(3)$ element.

Second, he introduced a covariant derivative (or, Ashtekar connection) ∇^A on Σ. As triads comprise the information on the metric, the covariant derivative contains that on the second fundamental form. For this, recall that the latter one is the quadratic form defined by the Weingarten mapping W with $W(X) := {}^4\nabla_X n$. Here, n is the normal to Σ within (M, g), and ${}^4\nabla$ is the Levi-Civita connection on (M, g). Now, the Ashtekar connection is defined by [30, 33]

$$\nabla^A_X Y := \nabla_X Y + \beta\, W(X) \times Y\,.$$

Here, the vector product has been transferred from $\mathbb{R}^3$ to $T\Sigma$ using a q-orthonormal triad. The complex number β is a parameter [15, 42] of the theory and is called Barbero-Immirzi parameter.

Ashtekar observed that the connection and the triad form a canonical pair of variables. At the same time, there appeared an additional constraint, the so-called Gauß constraint that originates in the gauge freedom introduced via replacing metrics by triads. This, however, is no big deal as now, having connections as

[7] Alternatively, one can also consider the space of all Riemannian 3-metrics modulo diffeomorphisms. This leads to the so-called superspace. However, its mathematical structure is rather complicated [36].

variables, we are in the realm of gauge field theories. There, gauge invariance as incorporated by the Gauß constraint can be tamed rather easily. The big advantage of the original Ashtekar variables became apparent, when the Hamilton constraint was calculated: for $\beta = \pm\mathrm{i}$, it is polynomial. This triggered the hope for a successful and rigorous canonical quantization of pure general relativity. However, as physical theories shall produce real numbers rather than complex ones, the choice of $\beta = \pm\mathrm{i}$ forced Ashtekar to introduce quite complicated reality conditions. It took about 10 years until Thiemann [51, 52] realized that the non-polynomiality which had remained for $\beta \neq \pm\mathrm{i}$, can be expressed by means of the Poisson bracket and some appropriate volume function.

For our purposes, however, these considerations are less relevant. We are going to study the configuration space only – neither the phase space nor the constraints. Thus, the main lesson we should keep in mind, is: general relativity, using Ashtekar's variables, can be formulated as a gauge field theory, i.e., its configuration space is spanned by the covariant derivatives on $T\Sigma$. Alternatively, one can consider $T\Sigma$ as an vector bundle that is associated to any[8] spin bundle over Σ. The latter one is always an $SU(2)$ principal fiber bundle over Σ. Its connections are in one-to-one correspondence with covariant derivatives on the tangent bundle over Σ. – To summarize:

Definition 10 Let G be a connected compact Lie group, let M be some manifold, and let P be some G-principal fiber bundle over M. Then $\mathcal{A}$ denotes the set of all connections in P.

Now, the **classical configuration space** of canonical general relativity is the set of all connections in an $SU(2)$ principal fiber bundle over some 3-dimensional manifold. Until the end of this section, however, we will not restrict ourselves to $G = SU(2)$ and $\dim M = 3$, but use $\mathcal{A}$ in the broader sense of the definition above.

Remark 11

1. Notably, for $\beta \neq \pm\mathrm{i}$, the resulting gauge theory does no longer correspond to a *space-time* gauge field theory, as the Ashtekar connection cannot be extended to a full space-time connection [49].
2. Neither for gravity nor for cosmology we will discuss the issue of gauge transforms, although the space of connections modulo gauge transforms usually serves as configuration space of gauge theories. However, a careful implementation of gauge transforms into our framework is still lacking. Nevertheless, we do not expect severe problems. But, the presentation would probably be much more technical, whence we would have focused just on spaces of connections anyway.

[8] There are spin structures, hence spin bundles, as Σ is orientable [43].

3.2 Quantum Configuration Space

Having settled the classical configuration space $\mathcal{A}$ for general relativity, we now have to select an appropriate algebra of functions on $\mathcal{A}$. Here, the motivation comes from lattice gauge field theories. There, rather than connections themselves, one considers parallel transports along the bonds of a lattice that is typically cubic. Here, we will now consider parallel transports just along arbitrary paths. Indeed, one can reconstruct a connection as soon as one knows all of its parallel transports.

Using all parallel transports, however, is technically a bit more subtle than in usual lattice gauge field theory. There, one always (at least implicitly) assumes to be given some (possibly global) trivialization of the bundle. This allows parallel transports to be just elements of the structure group. Actually, parallel transports are mappings $h_{\gamma,A} : P_{\gamma(0)} \longrightarrow P_{\gamma(1)}$ from the fiber over the starting point to the fiber over the end point of the path γ under consideration. Of course, each fiber is (non-canonically) isomorphic to the structure group G; for instance, choosing $\nu(m)$ in the fiber P_m over m, we get such an isomorphism $G \longrightarrow P_m$ via $g \longmapsto \nu(m)g$. Only now, as the mappings $h_{\gamma,A}$ commute with the right action of the structure group, one can identify them with elements of G via $h_{\gamma,A}(\nu(\gamma(0))) = \nu(\gamma(1))h^s_\gamma(A)$. Here, the set-theoretic global section[9] $\nu : M \longrightarrow P$ is any function with $\pi \circ \nu = \mathrm{id}_M$ for $\pi : P \longrightarrow M$ the canonical projection.

Considering parallel transports as elements in G rather than equivariant mappings between fibers, indeed, is much more convenient for our purposes. In fact, as G is assumed compact, h^ν_γ can now be considered as a mapping from $\mathcal{A}$ to G, whose matrix element functions are bounded functions on $\mathcal{A}$ – exactly the structures we need for our algebra.

Definition 12 Fix some set-theoretic global section in P and let $\mathfrak{B}$ contain precisely the functions $f \circ h^\nu_\gamma : \mathcal{A} \longrightarrow \mathbb{C}$, with $f : G \longrightarrow \mathbb{C}$ running over the matrix functions[10] and γ running over all analytic paths in M. Then $\mathfrak{A}$ is set to be the unital C^*-subalgebra of $\ell^\infty(\mathcal{A})$ generated by $\mathfrak{B}$.

In the loop quantum gravity literature, $\mathfrak{B}$ (or, often, some slightly larger subsets of $\mathfrak{A}$) is usually referred to as the set of cylindrical functions. Note that $\mathfrak{A}$ does not depend on the choice of the set-theoretic section ν. In fact, if μ is another section, there are some $g_x, g_y \in G$, such that $h^\nu_\gamma(A) = g_y^{-1} h^\mu_\gamma(A) g_x$ for all A and all γ connecting x and y. Now, it is clear that we get the same $\mathfrak{A}$ in both situations. In the following, we will tacitly assume to have fixed some set-theoretic section for calculating parallel transport functions, and simply write h_γ instead of h^ν_γ.

[9] Note that we do not require ν to even be a local section in the bundle sense. In fact, ν need not be continuous; this is referred to by noting "set-theoretic" [26].

[10] We assume to have fixedly chosen G as a Lie subgroup of some $U(n)$.

According to Sect. 2, now the **quantum configuration space** of canonical general relativity in the loop approach is the spectrum of $\mathfrak{A}$. This is a compact Hausdorff space and denoted by $\overline{\mathcal{A}}$. Its elements are called generalized connections. By Proposition 1_2 it contains $\mathcal{A}$ as a dense subspace.

3.3 Groupoid Homomorphisms

At a first glance, spectra of abelian C^*-algebras need not look easily accessible. This, however, is not true for the set $\overline{\mathcal{A}}$ of generalized connections.

For this, let us go back to the case of "classical" connections or better their parallel transports. So far, we have always considered them as functions from $\mathcal{A}$ to G, indexed by the paths in M. Now, we will consider them as mappings $h_A : \mathcal{P} \longrightarrow G$ from the set $\mathcal{P}$ of paths to G indexed by the connections. Of course, h_A will be smooth in a certain sense, but that is not the property most relevant for us. Instead, h_A is multiplicative. In fact, given a path γ cut in two pieces γ_1 and γ_2, the parallel transports obey $h_A(\gamma) \equiv h_A(\gamma_1\gamma_2) = h_A(\gamma_1)h_A(\gamma_2)$. Similarly, $h_A(\gamma^{-1}) = h_A(\gamma)^{-1}$, for γ^{-1} being the path γ passed in the opposite direction. Thus, giving the set $\mathcal{P}$ of analytic paths the structure of a groupoid,[11] each h_A is a homomorphism from $\mathcal{P}$ to G. And this is the key to the spectrum, giving

Proposition 13 *$\overline{\mathcal{A}}$ is isomorphic to* $\mathrm{Hom}(\mathcal{P}, G)$.

This means, $\overline{\mathcal{A}}$ consists of *all* homomorphisms, not just the sort-of-smooth ones. The isomorphism itself is rather simply described. For this, note that we may extend $\overline{A} \in \overline{\mathcal{A}}$ to

$$\overline{A} \quad : \quad \mathfrak{A} \otimes \mathbb{C}^{n\times n} \longrightarrow \mathbb{C}^{n\times n},$$

with our compact G embedded into $U(n) \subseteq \mathbb{C}^{n\times n}$. Then we just have

$$\overline{A}(h_\gamma) = \overline{A}(\gamma),$$

where the right-hand $\overline{A} : \mathcal{P} \longrightarrow G$ is the homomorphism that corresponds to the left-hand $\overline{A} \in \overline{\mathcal{A}}$ (extended as above). That the mapping above is indeed an isomorphism follows from the homomorphy of parallel transports, and as h_γ equals h_δ iff γ and δ coincide up to the parametrization.

We will identify $\overline{\mathcal{A}}$ and $\mathrm{Hom}(\mathcal{P}, G)$ in the following.

[11] For this, one has to identify paths that coincide up to their parametrization.

3.4 Projective Limits

Beyond the formulations of $\overline{\mathcal{A}}$ via C^*-algebras and via path groupoids, there is a third one using projective limits. For this, consider any analytic graph $\boldsymbol{\gamma}$, i.e., a finite graph whose edges are analytic paths γ_i. Any such $\boldsymbol{\gamma}$ defines a surjective continuous mapping $h_{\boldsymbol{\gamma}} : \overline{\mathcal{A}} \longrightarrow G^n$ via $h_{\boldsymbol{\gamma}}(\overline{A}) = (\overline{A}(\gamma_1), \ldots, \overline{A}(\gamma_n))$. These mappings $h_{\boldsymbol{\gamma}}$ can be seen as canonical projections of an appropriate projective limit.

Indeed, we define an ordering on the set of analytic paths as follows. We say $\boldsymbol{\gamma} \leq \boldsymbol{\delta}$ iff any edge in $\boldsymbol{\gamma}$ can be decomposed into edges of $\boldsymbol{\delta}$ or their inverses. Corresponding to these decompositions, we define a projection

$$\pi^{\boldsymbol{\delta}}_{\boldsymbol{\gamma}} : G^{\#\boldsymbol{\delta}} \longrightarrow G^{\#\boldsymbol{\gamma}} .$$

For instance, if $\gamma_1 = \delta_1\delta_2$ and $\gamma_2 = \delta_3^{-1}$, then $\pi^{\boldsymbol{\delta}}_{\boldsymbol{\gamma}}(g_1, g_2, g_3) = (g_1 g_2, g_3^{-1})$. As

$$\pi^{\boldsymbol{\delta}}_{\boldsymbol{\gamma}} \circ \pi^{\boldsymbol{\varepsilon}}_{\boldsymbol{\delta}} = \pi^{\boldsymbol{\varepsilon}}_{\boldsymbol{\gamma}} \qquad \text{for } \boldsymbol{\gamma} \leq \boldsymbol{\delta} \leq \boldsymbol{\varepsilon},$$

these mappings form a projective system. One can easily show that

Proposition 14 *$\overline{\mathcal{A}}$ is homeomorphic to $\varprojlim_{\boldsymbol{\gamma}} G^{\boldsymbol{\gamma}}$ via $\overline{A} \longmapsto \big(h_{\boldsymbol{\gamma}}(\overline{A})\big)_{\boldsymbol{\gamma}}$.*

In particular, the canonical projections of the projective limit are just the $h_{\boldsymbol{\gamma}}$.

3.5 Ashtekar-Lewandowski Measure

One of the main breakthroughs of loop quantum gravity was not only the definition of a compact quantum configuration space for general relativity, but even more the rigorous construction of a normalized Radon measure thereon, namely the Ashtekar-Lewandowski measure. Its construction is very easy using the projective limit framework, given the underlying ordering is directed which is the case for analytic graphs. Recall that then the normalized Radon measures on a projective limit are in one-to-one correspondence to consistent families of normalized Radon measures on the constituents of the limit. In our case, this means that the measures on $\overline{\mathcal{A}}$ correspond to families $(\mu_{\boldsymbol{\gamma}})_{\boldsymbol{\gamma}}$ of measures on the $G^{\#\boldsymbol{\gamma}}$ that fulfill

$$\mu_{\boldsymbol{\gamma}} = (\pi^{\boldsymbol{\delta}}_{\boldsymbol{\gamma}})_* \mu_{\boldsymbol{\delta}} \qquad \text{for all } \boldsymbol{\gamma} \leq \boldsymbol{\delta}.$$

The most obvious choice is to let each $\mu_{\boldsymbol{\gamma}}$ be the normalized Haar measure. Indeed, this family is consistent and corresponds to the Ashtekar-Lewandowski measure μ_{AL}. This measure underlies all the constructions in loop quantum gravity. In particular, it provides us with a kinematical Hilbert space $L^2(\overline{\mathcal{A}}, \mu_{\mathrm{AL}})$.

Of course, there are many more measures on $\overline{\mathcal{A}}$, but the choice of the Ashtekar-Lewandowski measure is indeed natural. There are strong uniqueness results that single out μ_{AL}. In particular, up to some technical assumptions like regularity and cyclicity, both the holonomy-flux algebra [44] and the Weyl algebra [29] can be represented only on $L^2(\overline{\mathcal{A}}, \mu_{\mathrm{AL}})$ in a diffeomorphism-covariant way.

3.6 Explicit Example

Having laid out the theory, we should show that we have made a nontrivial extension of the classical configuration space. So let us explicitly construct generalized, but non-smooth connections. For this, fix some path δ as well as some $g \in G$, and let $n(\gamma)$ tell us how often γ passes an initial segment of δ (counted negatively if passed in the other direction). Now, $\overline{A}_g(\gamma) := g^{n(\gamma)}$ is a well-defined generalized connection. If, for simplicity, we assume P to be trivial, then it is a smooth connection iff $g = \mathbf{1}$, showing that $\mathcal{A}$ is properly contained in $\overline{\mathcal{A}}$. For general P, the argumentation is similar.

3.7 Paths

When defining $\overline{\mathcal{A}}$ to be the quantum configuration space, we have assumed without further comment that the algebra $\mathfrak{A}$ is generated by the parallel transport functions along all analytic paths in M. Why have we done this? Why have we not used further paths? Why have we not restricted ourselves to smaller classes?

Well, first of all, analytic objects behave very nicely. Indeed, if two analytic paths have infinitely many intersection points, they have to coincide on full intervals which may even be taken maximal. This implies that two analytic graphs are always subgraphs of a third analytic graph, i.e., the ordering on analytic graphs introduced above is direct. This has turned out crucial for the construction of measures.

Of course, one has to grant that one can weaken the smoothness requirements the paths are to fulfill. For that purpose, webs [13, 14, 27, 28] in the smooth category or hyphs [25] in the arbitrary C^k categories have been introduced and widely studied. Indeed, significant parts of the theory have been transferred. Nevertheless, the use of paths that are non-analytic, has lead to enormous technical difficulties. Thus, it is at least a matter of convenience to choose the analytic category for all the manifolds, bundles, and paths in the game.

Conceptually, there is even a further justification for choosing analytic paths. Actually, general relativity seems to contradict analyticity, as the former one is a local, the latter one a non-local structure. However, this puzzle can be resolved using semianalytic structures [29, 40, 44, 45] rather than analytic ones. Indeed, semianalyticity provides us with non-local, i.e. non-rigid structures. Even more,

the loop quantum gravity uniqueness theorems mentioned above work in the semianalytic framework. For paths, semianalytic just means piecewise analytic, which is the same as to admit the concatenation of analytic paths. At the same time, the C^*-algebra $\mathfrak{A}$ generated by the analytic paths is the same as those generated by piecewise analytic paths. Therefore, at the level of graphs it is completely justified to restrict oneself to analytic paths.

It remains to discuss whether we might further restrict the set of paths, say to straight lines when the base manifold is $\mathbb{R}^3$. Indeed, there is no obstruction to do this. One just has to guarantee that with any admissible path all of its subpaths as well as its inverse are admissible. These issues will become relevant in cosmological models and will be discussed in more detail in Sect. 4.5.

4 Homogeneous Isotropic Loop Quantum Cosmology

Now we are going to apply our results to the case of $k = 0$ homogeneous isotropic cosmology. After recalling the implications of homogeneity and isotropy as well as explaining k, we will state the space of classical invariant connections. Then we will investigate the algebra of functions whose spectrum can be continuously embedded into the full space of generalized connections, in the analytic case. We also discuss other smoothness categories focusing on their embedding properties. Afterwards, we review the invariance of measures and close with the noncommutativity of symmetry reduction and quantization.

4.1 Euclidean Group Action

In general, homogeneity and isotropy imply that the sectional curvature k of the metric on the Cauchy surface Σ is constant [54]. If k even vanishes, then Σ is necessarily covered by $\mathbb{R}^3$. As we will assume that the Cauchy surface is even simply connected, Σ equals the Euclidean $\mathbb{R}^3$. Homogeneity and isotropy now mean that our theory shall be invariant under all rigid motions, hence w.r.t. the connected component E of the Euclidean group in 3 dimensions.

As we are going to study gravity and cosmology in their formulations using Ashtekar variables, we have to consider now connections in an $SU(2)$-principal fiber bundle P over $\Sigma = \mathbb{R}^3$. As Σ is contractible, the bundle is trivial, hence $P = \Sigma \times SU(2)$. The delicate point is how to lift the action of the Euclidean group from Σ to P and to the connections in P. The action on the Σ-part, of course, remains to be the defining action of the Euclidean group E. But, how to act on the $SU(2)$-part? Here, one should assume that not only E is acting, but even its covering group, which is homeomorphic to $\mathbb{R}^3 \times \mathrm{S}^3$. Finally, this leads to the following situation [38]:

Definition 15 The **symmetry group** of $k = 0$ homogeneous isotropic cosmology is

$$S = \mathbb{R}^3 \rtimes SU(2)\,.$$

It acts from the left on $P = \mathbb{R}^3 \times SU(2)$ via

$$(x, r) \circ (y, g) \longmapsto (ry + x, rg)\,.$$

Here, $SU(2)$ acts on $\mathbb{R}^3$ via first projecting $SU(2)$ to $SO(3)$ by the covering map. More explicitly, we have $[ry]^i \tau_i = \mathrm{Ad}_r(y^j \tau_j)$ for any $\mathfrak{su}(2)$ basis $\{\tau_i\}$ with $[\tau_i, \tau_j] = \varepsilon_{ij}^m \tau_m$.

4.2 Invariant Connections

In the next step, we have to identify the elements of $\mathcal{A}_{\mathrm{red}}$, i.e. the connections in P that are invariant under the action of the symmetry group S on P.

Proposition 16 *$\mathcal{A}_{\mathrm{red}}$ is isomorphic to $\mathbb{R}$. More precisely,*

$$\mathcal{A}_{\mathrm{red}} = \{\theta + \mathbf{c}\,\eta \mid \mathbf{c} \in \mathbb{R}\}$$

with θ being the Maurer-Cartan form on $G = SU(2)$ and with η being the $\mathfrak{su}(2)$-valued one-form on P given by

$$\eta_{(x,g)} = \mathrm{Ad}_g\, \tau_i \otimes \mathrm{d}x^i \quad \textit{for all } (x, g) \in P\,.$$

That the forms above are indeed invariant forms, can be calculated immediately. More elaborate is the proof that there are not any other invariant forms [38].

The more common version of the forms above is given by their pullbacks $\mathbf{c}\,\tau_i \otimes \mathrm{d}x^i$ to the base manifold using the canonical section into the trivial bundle $P = \mathbb{R}^3 \times SU(2)$.

4.3 Quantizing Algebra

Recall that we are aiming at constructing a version of loop quantum cosmology whose configuration space can be embedded into that of full loop quantum gravity. Therefore, we have to define the cosmological cylindrical functions as the restrictions of the gravitational cylindrical functions (see Definition 12) to $\mathcal{A}_{\mathrm{red}} \subseteq \mathcal{A}$. For this, let us study first how parallel transports depend on $\mathcal{A}_{\mathrm{red}}$.

Let there be given a connection $A \in \mathcal{A}$. We identify A with the corresponding connection one-form on M that one gets via pullback along the standard section in P; recall that P is trivial. Moreover, let $\gamma : [0,1] \longrightarrow M$ be some path in M and let γ_t be its restriction to $[0,t]$. Finally, denote by $\boldsymbol{g}(t) := h_A(\gamma_t)$ the parallel transport along γ_t. Then $\boldsymbol{g}$ obeys the differential equation

$$\dot{\boldsymbol{g}} = -A(\dot{\gamma})\,\boldsymbol{g} \qquad \text{with} \qquad \boldsymbol{g}(0) = \mathbf{1}\,. \tag{3}$$

Specializing to $\theta + \mathbf{c}\eta \in \mathcal{A}_{\mathrm{red}} \cong \mathbb{R}$, any matrix function a of $\boldsymbol{g}$ fulfills [21]

$$\ddot{a} + \mathbf{c}^2 a = \mathbf{c} f_0 a + f_1 \dot{a} \tag{4}$$

for certain $f_0, f_1 \in C[0,1]$ that can be expressed using $\dot{\gamma}$; moreover, $a(0) \in \mathbb{C}$ and $\dot{a}(0) \in \mathbb{C} + \mathbf{c}\mathbb{C}$ depend on γ. One can show that f_0 and f_1 vanish iff γ is a straight line; they are constant iff γ is a spiral arc, comprising the cases of straight lines and circles [21, 23].

In particular, we have now learned that the cosmological, i.e. reduced quantizing algebra $\mathfrak{A}_{\mathrm{red}}$ is generated by the functions $\mathbf{c} \longmapsto a(t)$, whereas a solves (4), t runs over $[0,1]$, and γ (which determines coefficients and initial values for (4)) runs over all analytic paths in $\mathbb{R}^3$. Note that a, of course, depends on $\mathbf{c}$ via (4).

Let us calculate $\mathfrak{A}_{\mathrm{red}}$. First consider straight lines. Here, (4) has the simple form $\ddot{a} + \mathbf{c}^2 a = 0$. Hence, $a(t)$ is a linear combination of $\mathrm{e}^{\mathrm{i}t\mathbf{c}}$ and $\mathrm{e}^{-\mathrm{i}t\mathbf{c}}$. Carefully handling the possible initial values, we see that any character $\mathbf{c} \longmapsto \mathrm{e}^{\mathrm{i}t\mathbf{c}}$ is contained in $\mathfrak{A}_{\mathrm{red}}$. If, next, we look at circles with radius $1/(2\lambda)$, (4) leads to $\ddot{a} + (\mathbf{c}^2 + \lambda^2)a = 0$ (after some t-dependent rescaling of a, irrelevant for our purposes). Its solutions a can be written as a linear combination of exponentials of $\pm \mathrm{i}t\sqrt{\mathbf{c}^2 + \lambda^2}$. Focusing on their $\mathbf{c}$-dependence, we see that for large $\mathbf{c}$ they behave like periodic functions. A more careful investigation shows that $a(t)$ is indeed a linear combination of a character of $\mathbb{R}$ and a function vanishing at infinity. Again, exhausting all $\lambda > 0$ and handling the initial values properly, we see that we can even approximate any sum of this type. This shows that $\mathfrak{A}_{\mathrm{red}}$ at least contains $C_{\mathrm{AP}}(\mathbb{R}) + C_0(\mathbb{R})$, i.e. all sums of an almost periodic function and a function vanishing at infinity. It is not very difficult, but technically a bit more elaborate to show that these sums even comprise all possibilities [23]:

Proposition 17 *The **quantizing algebra** for loop quantum cosmology is*

$$\mathfrak{A}_{\mathrm{red}} = C_0(\mathbb{R}) + C_{\mathrm{AP}}(\mathbb{R})\,.$$

Note that $\mathfrak{A}_{\mathrm{red}}$ is indeed a C^*-algebra [33, 46].

4.4 Generalized Invariant Connections

Our next task is to determine the spectrum $\overline{\mathbb{R}} \equiv \overline{\mathcal{A}_{\mathrm{red}}}$ of $\mathfrak{A}_{\mathrm{red}}$ [31]. If the sum of $C_0(\mathbb{R})$ and $C_{\mathrm{AP}}(\mathbb{R})$ was direct in the sense of C^*-algebras, this would be an easy game. However, obviously, this is not the case; the sum is only direct in the sense of vector spaces. Nevertheless, there is a bit beyond nothing. Indeed, observe that both algebras are C^*-subalgebras of $\ell^\infty(\mathbb{R})$ with $C_0(\mathbb{R})$ even being an ideal. This already suffices to show that the spectrum of $\mathfrak{A}_{\mathrm{red}}$ *as a set* equals the disjoint sum of the two single spectra, namely $\mathbb{R}$ and the Bohr compactification $\mathbb{R}_{\mathrm{Bohr}}$, respectively. To see this, define

$$\tau(\mathbf{c}) : a_0 + a_1 \longmapsto a_0(\mathbf{c}) + a_1(\mathbf{c}) \tag{5}$$

$$\tau(\mathbf{b}) : a_0 + a_1 \longmapsto \mathbf{b}(a_1) \tag{6}$$

for $\mathbf{c} \in \mathbb{R}$, $\mathbf{b} \in \mathbb{R}_{\mathrm{Bohr}} \equiv \operatorname{spec} C_{\mathrm{AP}}(\mathbb{R})$, $a_0 + a_1 \in C_0(\mathbb{R}) + C_{\mathrm{AP}}(\mathbb{R})$. From

$$\begin{aligned}
[\tau(\mathbf{b})]\big((a_0 + a_1)(b_0 + b_1)\big) &= [\tau(\mathbf{b})]\big((a_0 b_0 + a_0 b_1 + a_1 b_0) + a_1 b_1\big) \\
&= \mathbf{b}(a_1 b_1) \quad = \quad \mathbf{b}(a_1)\, \mathbf{b}(b_1) \\
&= [\tau(\mathbf{b})](a_0 + a_1)\, [\tau(\mathbf{b})](b_0 + b_1)
\end{aligned}$$

we see that $\tau : \mathbb{R} \sqcup \mathbb{R}_{\mathrm{Bohr}} \longrightarrow \overline{\mathbb{R}}$ is well defined. It is not very difficult to show that τ is even bijective, whence we will identify $\overline{\mathbb{R}}$ with $\mathbb{R} \sqcup \mathbb{R}_{\mathrm{Bohr}}$.

The determination of the topology of $\mathbb{R}$, however, is more elaborate [31]. As the sum of $C_0(\mathbb{R})$ and $C_{\mathrm{AP}}(\mathbb{R})$ is not direct, we cannot expect the topology to be the disjoint-sum topology. Indeed, it is not. Instead, it is twisted. It is generated by the following types of sets:

Type 1:	$V \sqcup \varnothing$	with open $V \subseteq \mathbb{R}$
Type 2:	$\complement K \sqcup \mathbb{R}_{\mathrm{Bohr}}$	with compact $K \subseteq \mathbb{R}$
Type 3:	$a_1^{-1}(U) \sqcup \tilde{a}_1^{-1}(U)$	with open $U \subseteq \mathbb{C}$ and $a_1 \in C_{\mathrm{AP}}(\mathbb{R})$.

Nevertheless, the relative topologies on $\mathbb{R}$ and $\mathbb{R}_{\mathrm{Bohr}}$ considered as subsets of $\overline{\mathbb{R}}$ are the usual ones. Also, $\mathbb{R}$ is open and dense in $\overline{\mathbb{R}}$. Moreover, the canonical mapping $\iota_{\mathrm{red}} : \mathbb{R} \longrightarrow \overline{\mathbb{R}} \equiv \mathbb{R} \sqcup \mathbb{R}_{\mathrm{Bohr}}$ is the identity on $\mathbb{R}$. Finally, as $\mathfrak{A}_{\mathrm{red}}$ is unital, $\overline{\mathbb{R}}$ is compact as desired.

4.5 Embeddings

By construction, $\overline{\mathbb{R}}$ is continuously embedded into $\overline{\mathcal{A}}$ extending the natural embedding of $\mathbb{R} \equiv \mathcal{A}_{\mathrm{red}}$ into $\mathcal{A}$. In fact, as we have defined $\mathfrak{A}_{\mathrm{red}}$ to be generated by

the parallel transport matrix functions restricted to $\mathcal{A}_{\mathrm{red}}$, the embedding criterion of Corollary 7 is fulfilled automatically. However, there are also other versions of loop quantum cosmology that have been discussed in the literature. They differ from our strategy by using different quantizing algebras. Indeed, the original way Bojowald invented loop quantum cosmology was to consider parallel transports along straight lines only. As we have seen above, these functions span the algebra of almost periodic functions whose spectrum is $\mathbb{R}_{\mathrm{Bohr}}$. However, $C_{\mathrm{AP}}(\mathbb{R})$ does *not* fulfill the embedding criterion of Corollary 7. In fact, we have seen that $\mathfrak{A}|_{\mathcal{A}_{\mathrm{red}}}$ is *not* contained in $C_{\mathrm{AP}}(\mathbb{R})$ although that is a necessary condition for embeddability.

Of course, these arguments are only valid assuming that the quantizing algebra for loop quantum gravity is indexed by all analytic graphs. Over the years, however, several other choices have been discussed: smooth paths [13, 14, 27], C^k paths [25], piecewise linear paths [22, 56], paths in a fixed graph [35], or paths given by iterated barycentric subdivisions [1]. Similarly, in the cosmological arena piecewise linear paths [19, 22], parts of a fixed geodesic [19] or just two paths having incommensurable lengths [53] have been investigated. We have displayed in Table 1 for each combination whether the classical embedding $\mathcal{A}_{\mathrm{red}} \subseteq \mathcal{A}$ does lift to the quantum level (+) or does not (−). Note that we have excluded the gravity cases based on a fixed graph or barycentric subdivisions, as there the quantizing algebras do, in general, not separate the classical configuration space [23], whence $\iota : \mathcal{A} \longrightarrow \overline{\mathcal{A}}$ is not injective there. It should now be no surprise that a continuous embedding is given if and only if the classes of paths used for the gravitational and for the cosmological theories coincide [23].

Consequently, the strategy presented above, i.e. defining the quantized algebras for gravity and cosmology using identical sets of paths is the only way to get embeddability. This, however, does not tell us a priori whether the choice for cosmology should follow that for gravity or vice versa. Indeed, in order to keep Bojowald's original straight-line cosmology, it has been argued [22] that one should restrict oneself to straight lines already at gravity level. We, however, think that this is not desirable as then other symmetries might not be treatable within full gravity. Therefore, we prefer our strategy "cosmology follows gravity".

Table 1 Continuous embeddings of quantum configuration spaces

Paths for... ...gravity \ ...cosmology	As for gravity	Piecewise linear	In a geodesic	Incommens'ble
Piecewise analytic	+	−	−	−
Piecewise smooth	+	−	−	−
Piecewise C^k	+	−	−	−
Piecewise linear	+	+	+	−

4.6 Invariant Measures

In order to define a kinematical Hilbert space and to then obtain quantum states, one should look for finite measures on the respective quantum configuration space. For full gravity, the Ashtekar-Lewandowski measure μ_{AL} on $\overline{\mathcal{A}}$ turned out to be the measure distinguished by strong uniqueness results [29, 44]. In Bojowald's cosmology, the Haar measure on $\mathbb{R}_{\mathrm{Bohr}}$ adopted that role [4]. What could now be the measure of choice in our version of loop quantum cosmology?

Well, the easiest way would be to choose a Haar measure on the quantum configuration space $\overline{\mathbb{R}} = \mathbb{R} \sqcup \mathbb{R}_{\mathrm{Bohr}}$. However, as Hanusch [39] pointed out, $\overline{\mathbb{R}}$ does not carry the structure of a topological group compatible with that on $\mathbb{R}$. No group structure – no Haar measure.

Thus, maybe we should lower our sights. Indeed, a Haar measure does not exploit the full structure of a topological group. Instead, it is defined to be invariant w.r.t. the left translation of the group on itself. For the Bohr compactification, we even need less than full invariance:

Lemma 18 *Any finite $\mathbb{R}$-invariant Radon measure on $\mathbb{R}_{\mathrm{Bohr}}$ is already $\mathbb{R}_{\mathrm{Bohr}}$-invariant.*

Proof Let U be a neighborhood in $\mathbb{R}_{\mathrm{Bohr}}$ of some compact K that fulfills $\mu(U) < \mu(K) + \varepsilon$, and let $\mathbf{b} \in \mathbb{R}_{\mathrm{Bohr}}$. By denseness of $\mathbb{R}$ in the compact group $\mathbb{R}_{\mathrm{Bohr}}$, there is some $\mathbf{c} \in \mathbb{R}$ with $\mathbf{b} + K \subseteq \mathbf{c} + U$, whence by $\mathbb{R}$-invariance

$$\mu(\mathbf{b} + K) \;\leq\; \mu(\mathbf{c} + U) \;=\; \mu(U) \;<\; \mu(K) + \varepsilon\,.$$

This gives $\mu(\mathbf{b} + K) = \mu(K)$. Now the proof follows from regularity. □

On the other hand, using the general strategy from Sect. 2.4, the $\mathbb{R}$-action on $\mathbb{R}_{\mathrm{Bohr}}$ can be considered as the lift of the standard $\mathbb{R}$-action on $\mathbb{R}$. For this, just observe that $\mathbb{R}_{\mathrm{Bohr}}$ is nothing but the quantum configuration space for $\mathcal{X} = \mathbb{R}$ and quantizing algebra $C_{\mathrm{AP}}(\mathbb{R})$. But, why should we look for $\mathbb{R}$-invariant measures at all? Well, for the same reason as in full gravity. In fact, the Ashtekar-Lewandowski measure is invariant under all exponentiated fluxes. In cosmology, their counterpart is just translations by real numbers. Therefore, it is very natural to ask for $\mathbb{R}$-invariant measures in the cosmological case. The Haar measure, as shown above, is indeed the only candidate in Bojowald's construction of loop quantum cosmology; in fact, here the quantizing algebra has been $C_{\mathrm{AP}}(\mathbb{R})$. In our framework, however, the quantizing algebra is $\mathfrak{A}_{\mathrm{red}} = C_0(\mathbb{R}) + C_{\mathrm{AP}}(\mathbb{R})$. Do we get an $\mathbb{R}$-action there as well? Yes, of course. Theorem 8 tells us that the only condition is the $\mathbb{R}$-invariance of $\mathfrak{A}_{\mathrm{red}}$, which is obviously given. Even more, as the action preserves the direct sum $C_0(\mathbb{R}) + C_{\mathrm{AP}}(\mathbb{R})$, the restriction of the $\mathbb{R}$-action on $\overline{\mathbb{R}}$ to its components $\mathbb{R}$ and $\mathbb{R}_{\mathrm{Bohr}}$ coincides

with the respective standard action. Finally, $\mathbf{x} \longmapsto L_{\mathbf{x}}^* a$ which maps $\mathbb{R}$ to $\mathfrak{A}_{\mathrm{red}}$, is continuous for all $a \in \mathfrak{A}_{\mathrm{red}}$ [38], whence the $\mathbb{R}$-action on $\overline{\mathbb{R}}$ is continuous as well by the closing remark in Sect. 2.4.

Now, we are left with just a final observation: although the topology of $\overline{\mathbb{R}} = \mathbb{R} \sqcup \mathbb{R}_{\mathrm{Bohr}}$ is not that of the disjoint sum, the Borel algebra of $\overline{\mathbb{R}}$ *is* the disjoint sum of the Borel algebras of $\mathbb{R}$ and of $\mathbb{R}_{\mathrm{Bohr}}$. This implies that the finite Radon measures on $\overline{\mathbb{R}}$ are the sums of finite Radon measures on $\mathbb{R}$ and on $\mathbb{R}_{\mathrm{Bohr}}$ [31, 38].

Proposition 19 *The Haar measure on the $\mathbb{R}_{\mathrm{Bohr}}$-part is the only normalized Radon measure on $\overline{\mathbb{R}}$ that is $\mathbb{R}$-invariant [38].*

Proof Let $\mu = \mu_0 + \mu_1$ be such a measure on $\overline{\mathbb{R}} = \mathbb{R} \sqcup \mathbb{R}_{\mathrm{Bohr}}$. Setting $I = [0, 1)$, we have $1 \geq \mu_0(\mathbb{R}) = \sum_{n \in \mathbb{Z}} \mu_0(n + I) = \sum_{\mathbb{Z}} \mu_0(I)$ by $\mathbb{R}$-invariance, which implies $\mu_0 = 0$. As now μ_1 is $\mathbb{R}$-invariant, the proof follows from Lemma 18. □

This proposition has an astonishing consequence: it reconciles the original approach by Bojowald with that discussed here – both lead to the same kinematical Hilbert space. Our approach, however, has the advantage that it is functorial. This means that we can guarantee for a continuous embedding of the configuration spaces being a fundamental step in the Bojowald-Kastrup construction [20] of symmetric states in loop quantum gravity.

The bridge between loop quantum gravity and loop quantum cosmology that had been destroyed by the non-embedding results [21] of Brunnemann and the author, has now been rebuilt at another place.

4.7 Invariant Generalized Connections

So far, we have studied loop quantum cosmology as the quantum theory of the cosmological sector of gravity. In other words, we have first reduced the theory and then quantized. Does this give the same result as first quantizing and then reducing? In other words, is loop quantum cosmology the homogeneous isotropic sector of full loop quantum gravity?

From the general theory we know that we can lift the action of the classical symmetry group S on $\mathcal{A}$ to an action on $\overline{\mathcal{A}}$. The generalized connections that are invariant w.r.t. the lifted action form the space $\overline{\mathcal{A}}_{\mathrm{red}}$ which is a closed, hence compact subset of $\overline{\mathcal{A}}$. Considering $\overline{\mathcal{A}_{\mathrm{red}}}$ as a subset of $\overline{\mathcal{A}}$, we already know that $\overline{\mathcal{A}_{\mathrm{red}}}$ is a subset of $\overline{\mathcal{A}}_{\mathrm{red}}$ by Theorem 9. The final question of this section is now: do both spaces even coincide or not?[12]

[12]The results of Sects. 4.7 and 4.8 can, in principle, be found in the very voluminous and interesting thesis [38] by Hanusch. Here, however, we have drastically simplified and streamlined notations, statement presentations and proofs.

Invariant Homomorphisms

Before we will solve this problem in Sect. 4.8, we should first go back to the level of classical connections and re-consider the action of S on parallel transports. Using the fact that parallel transports (in the sense of mappings between fibers) commute with the right action of the structure group, it is a straightforward calculation that the action of S on $A \in \mathcal{A}$ gives

$$h_\gamma(\varphi_s^* A) = r^{-1}\, h_{s\gamma}(A) r \qquad \text{for all } s = (x, r) \in S \text{ and paths } \gamma \in \mathcal{P}.$$

As $\mathcal{A}$ is dense in $\overline{\mathcal{A}}$, the action of S lifts to an action on $\overline{\mathcal{A}} = \mathrm{Hom}(\mathcal{P}, G)$ with

$$\big[s \circ \overline{A}\big](\gamma) = r^{-1}\, \overline{A}(s\gamma)\, r \qquad \text{for all } s = (x, r) \in S \text{ and paths } \gamma \in \mathcal{P}.$$

Thus, we have determined the set $\overline{\mathcal{A}}_{\mathrm{red}}$ of S-invariant generalized connections:

Proposition 20 *A generalized connection $\overline{A} \in \overline{\mathcal{A}}$ is S-invariant iff*

$$\overline{A}(s\gamma) = r\overline{A}(\gamma)r^{-1} \tag{7}$$

for all $s = (x, r) \in S$ and all paths[13] *$\gamma \in \mathcal{P}$.*

Straight Lines

Let us study how the proposition above restricts the possible parallel transports along straight lines. First of all, observe that shifting any path by some fixed $\mathbb{R}^3$ element does not alter the parallel transport at all. Thus, we may restrict ourselves to the lines $\gamma_v(t) := tv$ through the origin (w.l.o.g., $v \neq 0$). Fix now some $\overline{A} \in \overline{\mathcal{A}}_{\mathrm{red}}$ and some $v \in \mathbb{R}^3$ and denote the parallel transport of $\overline{A}$ along γ_v from 0 to t by $\boldsymbol{g}(t)$. Using the just obtained shift invariance and the homomorphy property of generalized connections, we see that $\boldsymbol{g} : \mathbb{R} \longrightarrow SU(2)$ is a one-parameter subgroup of $SU(2)$. Observe, however, that $\boldsymbol{g}$ need *not* be continuous. As $\mathbb{R}$ is commutative, the image of $\boldsymbol{g}$ is abelian, hence contained in a maximal torus. This means, it factorizes into $\boldsymbol{g} = T \circ \mathbf{b}$ with $\mathbf{b} : \mathbb{R} \longrightarrow \mathrm{S}^1$ being a (possibly non-continuous) homomorphism, and $T : \mathrm{S}^1 \longrightarrow SU(2)$ (a Lie embedding of) a maximal torus in $SU(2)$. Using Pontryagin duality, we might identify $\mathbf{b}$ with an element of $\mathbb{R}_{\mathrm{Bohr}}$.

Can we further restrict the possible tori? Yes, we can. Observe that γ_v is stabilized by all $r \in SU(2)$ with $rv = v$. These elements correspond to rotations $\exp(tv^i\tau_i)$ around the axis defined by $v \neq 0$. They span a maximal torus T_v; seen as an

[13] In order not to overload the notation, we refrain from writing "paths modulo reparametrization", here and in the following. Indeed, it should be clear that and how the action of S transfers to these equivalence classes.

embedding, it is given by

$$T_v : \mathrm{S}^1 \longrightarrow SU(2) \qquad \text{with} \qquad T_v' = -\mathrm{i}v^i\tau_i.$$

By (7), however, this torus has to commute with all $\boldsymbol{g}(t)$. Thus, if we assume for a moment that $\boldsymbol{g}$ is not central this implies $T = T_v$. But, if $\boldsymbol{g}$ is central, we can and will choose $T = T_v$ as well. Altogether, we have $\boldsymbol{g} = T_v \circ \mathbf{b}$, and the only remaining freedom is the choice of $\mathbf{b}$.

Symmetries of Paths

It is now very desirable to learn more about the restrictions that (7) imposes on arbitrary paths. Basically, there are two constraints: first the requirement to have a homomorphism, and second to have an invariant one. For straight lines, we can see immediately their consequences: the first one implies that $\mathbf{b}$ has to be a homomorphism, the second one implies that the torus T must be T_v. Similar statements can also be found for several other curves; see, e.g., the thesis of Hanusch [38] for a comprehensive treatment.

There, Hanusch starts his investigations by exploiting the invariance relations first. The crucial question is: which paths are in some sense independent from each other? In other words, when can a path be mapped by some element of the symmetry group S to itself, or at least when do they overlap? For this, obviously, one has to investigate the symmetry behavior of analytic paths. Basically, there are (at least) two sort-of independent types [38].

1. There are paths γ that exhibit a continuous symmetry *(Lie paths)*.
   They are given by (subpaths of) $\gamma(t) = \mathrm{e}^{tX}x$ where X lies in the Lie algebra of S and x is in M. These are just the integral curves of the fundamental vector fields induced by the symmetry group action on M.
2. There are paths γ that exhibit a discrete symmetry *(brick paths)*.
   Here, we have (modulo the stabilizer of γ) at most finitely many elements $s \in S$ for which $s\gamma$ and γ share a common subpath. In particular, such a γ has a subpath that has no accumulation point with any of its S-translates.

Recently, the author of the present review has proven that these paths indeed comprise all possible types in the homogeneous isotropic case; even more, this statement remains true for all symmetry group actions that are pointwise proper and analytic [32]. Moreover, it is known [38] that the types above are stable w.r.t. decomposition and inversion of paths, and, of course, there is no symmetry mapping a path from one class into another. Therefore, the parallel transports can be assigned to paths in different classes completely independently (although there remain constraints within the classes), which induces a product structure on $\overline{\mathcal{A}}_{\mathrm{red}}$.

For the Lie curves, one can go even further. Indeed, also there one can introduce a notion of independence which tells us basically that the respective curves do not share full segments. Recall that any Lie curve is induced by some element in the Lie

algebra $\mathfrak{s}$ of S. Therefore, via independence, the algebraic relations in (7) induce an equivalence relation on $\mathfrak{s}$. As non-equivalent paths can be assigned parallel transports independently, this again refines the product structure of $\overline{\mathcal{A}}_{\mathrm{red}}$. Within the factors, the problem is reduced to the constraints on parallel transports of the respective equivalence class. Finally, Hanusch obtained

$$\overline{\mathcal{A}}_{\mathrm{red}} = \mathbb{R}_{\mathrm{Bohr}} \times \left[\mathbb{R}_{\mathrm{Bohr}} \tilde{\times} \mathrm{S}^1\right]^{\mathbb{R}\times\mathbb{R}_+} \times \overline{\mathcal{A}}^{\mathrm{brick}}_{\mathrm{red}}\,, \tag{8}$$

where $\sim$ indicates some sort of projectivation. Observe that the first factor $\mathbb{R}_{\mathrm{Bohr}}$ is exactly the freedom that has remained for choosing parallel transports along straight lines (see above). The other paths require a more elaborate discussion.

4.8 Reduction vs. Quantization

Finally, let us show that $\overline{\mathcal{A}}_{\mathrm{red}}$ is indeed larger than $\overline{\mathcal{A}_{\mathrm{red}}}$. The basic idea is to show that there are just two connections in $\overline{\mathcal{A}_{\mathrm{red}}}$ that have trivial parallel transports along all straight lines, but infinitely many in $\overline{\mathcal{A}}_{\mathrm{red}}$.

Let us begin with the parallel transports for generalized invariant connections. For this, let first $\mathbf{c} \in \mathbb{R}$ and denote the straight line connecting 0 and tv by γ_t. Recall that $\mathbf{c}$ corresponds to the smooth invariant connection $\sigma(\mathbf{c}) \equiv \theta + \mathbf{c}\eta \in \mathcal{A}_{\mathrm{red}}$, having local one-form $A = \mathbf{c}\tau_i \otimes \mathrm{d}x^i$, hence $A(\dot\gamma) = \mathbf{c}\dot\gamma^i\tau_i$. Thus, the corresponding parallel transport along γ_t is, by (3),

$$h_{\gamma_t}(\sigma(\mathbf{c})) = \mathrm{e}^{-\mathbf{c}tv^i\tau_i} \quad\equiv\quad T_v(\mathrm{e}^{-\mathrm{i}\mathbf{c}t}) \quad\equiv\quad T_v(\chi_{-t}(\mathbf{c}))\,. \tag{9}$$

For general $\overline{\mathbf{c}} \in \overline{\mathbb{R}}$, the parallel transport of $\overline{\sigma}(\overline{\mathbf{c}}) \in \overline{\mathcal{A}}_{\mathrm{red}}$ along γ_t is given by

$$\begin{aligned}
[\overline{\sigma}(\overline{\mathbf{c}})](\gamma_t) &= [\overline{\sigma}(\overline{\mathbf{c}})](h_{\gamma_t}) && (\overline{A}(\gamma) = \overline{A}(h_\gamma) \text{ as } \overline{\mathcal{A}} = \mathrm{Hom}(\mathcal{P}, G))\\
&= \overline{\mathbf{c}}(h_{\gamma_t} \circ \sigma) && (\overline{\sigma}(\overline{\mathbf{c}}) = \overline{\mathbf{c}} \circ \sigma^* \text{ by Lemma 5})\\
&= \overline{\mathbf{c}}(T_v \circ \chi_{-t}) && (\text{see (9)})\\
&= [T_v \circ \overline{\mathbf{c}}](\chi_{-t}) && (\text{algebras extended by } \mathbb{C}^{n\times n}).
\end{aligned}$$

This shows immediately that $0 \in \mathbb{R}$ and $0_{\mathrm{Bohr}} \in \mathbb{R}_{\mathrm{Bohr}}$ are the only elements in $\overline{\mathbb{R}}$ for which the parallel transports along all straight lines are $\mathbf{1}$ (see (5) and (6)).

Let us now turn to the construction of a bunch of invariant generalized connections having trivial parallel transports along all straight lines. For every homomorphism $\mathbf{b} : \mathbb{R} \longrightarrow \mathrm{S}^1$ define a generalized connection $\overline{A}_{\mathbf{b}}$ by

$$\overline{A}_{\mathbf{b}}(\gamma) := \begin{cases} \mathbf{1} & \text{if } \gamma \text{ does not pass a circular arc} \\ T_n(\mathbf{b}(t)) & \text{if } \gamma \text{ has length } t \text{ and rotates in direction } n. \end{cases}$$

Here, "in direction" n means that the rotation axis is parallel to n. Moreover, the "length" t is set negative if γ rotates according the left-hand rule.[14] As T_n and $\mathbf{b}$ are homomorphisms, $\overline{A}_{\mathbf{b}}$ is in $\overline{\mathcal{A}}$. In particular, it is trivial on all straight lines. However, it is also S-invariant: First, if γ is not circular, then neither does any $s\gamma$; hence both the parallel transports on γ and on $s\gamma$ are trivial, whence the invariance condition (7) is trivially fulfilled. Second, if γ rotates in direction n with length t, then $s\gamma$ rotates in direction rn with length t, as $s = (x, r) \in S$ is an isometry. Now, (7) follows as $T_{sn} = \mathrm{Ad}_r \circ T_n$. This shows that $\overline{A}_{\mathbf{b}}$ is in $\overline{\mathcal{A}}_{\mathrm{red}}$ for all $\mathbf{b}$. And now it is clear that there are more than two connections in $\overline{\mathcal{A}}_{\mathrm{red}}$ that are trivial along straight lines. This proves

Theorem 21 *We have* $\overline{\mathcal{A}_{\mathrm{red}}} \subset \overline{\mathcal{A}}_{\mathrm{red}}$.

Thus, we have shown for the homogeneous isotropic case:

Quantization and symmetry reduction do not commute.

5 Conclusions

In our article, we have reviewed the mathematical theory underlying the configuration space constructions of loop quantum gravity and loop quantum cosmology. Beginning with abstractly discussing the C^*-algebraic mathematical foundations of loop quantization in general, we have finally seen that loop quantization and symmetry reduction do not commute for homogeneous isotropic cosmology.

It is now natural to ask about other symmetries. Indeed, again Hanusch [38] has already obtained several, at least partial results for spherically symmetric, for homogeneous and for semihomogeneous cosmologies. He was able to calculate all smooth invariant connections [37]; for the spherically symmetric case, this required methods beyond the classical results by Wang [55] or Harnad, Shnider, Vinet [41]. In the other two cases, he was even able to prove again that quantization and reduction do not commute. Here, the proofs are technically more involved than for the homogeneous isotropic case. Besides, in all these cases, at least the invariant homomorphisms along Lie curves (cf. (8)) have been derived by Hanusch. This could make the definition of measures feasible not only on $\overline{\mathcal{A}_{\mathrm{red}}}$ as we showed here, but also on $\overline{\mathcal{A}}_{\mathrm{red}}$.

In general, configuration spaces are only a small part of the problem. The next one would be to study the full phase space. For loop quantum gravity, this lead to the holonomy-flux $*$-algebra and the Weyl C^*-algebra whose representation theory turned out to be fundamental. For homogeneous isotropic loop quantum cosmology, the result by Ashtekar and Campiglia [4] has similar relevance. However, their proof

[14] This way, rotation in direction n with length t equals rotation in direction $-n$ with length $-t$. The homomorphy property of $\mathbf{b}$ together with $T_{-n} = T_n^{-1}$ shows that $\overline{A}_{\mathbf{b}}(\gamma)$ is well defined.

relied on the Bojowald version of the configuration space. It is now natural to ask for an extension to the framework presented here. Indeed, one can expect to get similar uniqueness as the $\mathbb{R}$-invariance already singles out the same measure as in [4], namely the Haar measure on $\mathbb{R}_{\mathrm{Bohr}}$. Having done this, one should enter the final stage of the Bojowald-Kastrup program: the construction of symmetric quantum states.

But, even if we would be able to perform there well, there is still one conceptual issue left open. Indeed, any measure, any phase space, any uniqueness result above, rests upon one of the configuration spaces of loop quantum cosmology. But, typically, quantization and symmetry reduction do not commute. It is a completely open field to discuss all the questions above using the invariant configuration space of symmetric loop quantum gravity.

Acknowledgements The author is very grateful to the organizers of the Regensburg conference on quantum mathematical physics for the kind invitation. The author is also very grateful to Maximilian Hanusch for numerous discussions and helpful comments on a draft version of this article.

References

1. J. Aastrup, J.M. Grimstrup, R. Nest, On spectral triples in quantum gravity I. Class. Quantum Gravity **26**, 065011 (2009)
2. A. Ashtekar, New variables for classical and quantum gravity. Phys. Rev. Lett. **57**, 2244–2247 (1986)
3. A. Ashtekar, New Hamiltonian formulation of general relativity. Phys. Rev. **D36**, 1587–1602 (1987)
4. A. Ashtekar, M. Campiglia, On the uniqueness of Kinematics of loop quantum cosmology. Class. Quantum Gravity **29**, 242001 (2012)
5. A. Ashtekar, C.J. Isham, Representations of the holonomy algebras of gravity and nonabelian gauge theories. Class. Quantum Gravity **9**, 1433–1468 (1992)
6. A. Ashtekar, J. Lewandowski, in *Knots and Quantum Gravity* (Oxford University Press, Oxford, 1994), pp. 21–61
7. A. Ashtekar, J. Lewandowski, Differential geometry on the space of connections via graphs and projective limits. J. Geom. Phys. **17**, 191–230 (1995)
8. A. Ashtekar, J. Lewandowski, Projective techniques and functional integration for gauge theories. J. Math. Phys. **36**, 2170–2191 (1995)
9. A. Ashtekar, J. Lewandowski, Background independent quantum gravity: a status report. Class. Quantum Gravity **21**, R53–R152 (2004)
10. A. Ashtekar, J. Lewandowski, D. Marolf, J.M. Mourão, Th. Thiemann, Quantization of diffeomorphism invariant theories of connections with local degrees of freedom. J. Math. Phys. **36**, 6456–6493 (1995)
11. A. Ashtekar, M. Bojowald, J. Lewandowski, Mathematical structure of loop quantum cosmology. Adv. Theor. Math. Phys. **9**, 233–268 (2003)
12. A. Ashtekar, T. Pawlowski, P. Singh, Quantum nature of the big bang. Phys. Rev. Lett. **96**, 141301 (2006)
13. J.C. Baez, S. Sawin, Functional integration on spaces of connections. J. Funct. Anal. **150**, 1–26 (1997)

14. J.C. Baez, S. Sawin, Diffeomorphism-invariant spin network states. J. Funct. Anal. **158**, 253–266 (1998)
15. J.F. Barbero, Real Ashtekar variables for Lorentzian signature space-times. Phys. Rev. **D51**, 5507–5510 (1995)
16. A.N. Bernal, M. Sánchez, On smooth Cauchy hypersurfaces and Geroch's splitting theorem. Commun. Math. Phys. **243**, 461–470 (2003)
17. A.N. Bernal, M. Sánchez, Further results on the smoothability of Cauchy hypersurfaces and Cauchy time functions. Lett. Math. Phys. **77**, 183–197 (2006)
18. M. Bojowald, Absence of singularity in loop quantum cosmology. Phys. Rev. Lett. **86**, 5227–5230 (2001)
19. M. Bojowald, Isotropic loop quantum cosmology. Class. Quantum Gravity **19**, 2717–2742 (2002)
20. M. Bojowald, H.A. Kastrup, Quantum symmetry reduction for diffeomorphism invariant theories of connections. Class. Quantum Gravity **17**, 3009–3043 (2000)
21. J. Brunnemann, Ch. Fleischhack, On the configuration spaces of homogeneous loop quantum cosmology and loop quantum gravity. Math. Phys. Anal. Geom. **15**, 299–315 (2012)
22. J. Engle, Piecewise linear loop quantum gravity. Class. Quantum Gravity **27**, 035003 (2010)
23. Ch. Fleischhack, *Loop quantization and symmetry: configuration spaces*. e-print: 1010.0449 [math-ph]
24. Ch. Fleischhack, *Mathematische und physikalische Aspekte verallgemeinerter Eichfeldtheorien im Ashtekarprogramm (Dissertation)*, Universität Leipzig (2001)
25. Ch. Fleischhack, Hyphs and the Ashtekar-Lewandowski Measure. J. Geom. Phys. **45** 231–251 (2003)
26. Ch. Fleischhack, Regular connections among generalized connections. J. Geom. Phys. **47**, 469–483 (2003)
27. Ch. Fleischhack, Parallel transports in webs. Math. Nachr. **263–264**, 83–102 (2004)
28. Ch. Fleischhack, Proof of a conjecture by Lewandowski and Thiemann. Commun. Math. Phys. **249** 331–352 (2004)
29. Ch. Fleischhack, Representations of the Weyl algebra in quantum geometry. Commun. Math. Phys. **285**, 67–140 (2009)
30. Ch. Fleischhack, On Ashtekar's formulation of general relativity. J. Phys. (Conf. Ser.) **360**, 012022 (2012)
31. Ch. Fleischhack, Spectra of Abelian C^*-subalgebra sums. e-print: 1409.5273 [math.FA]
32. Ch. Fleischhack, Symmetries of analytic paths. e-print: 1503.06341 [math-ph]
33. Ch. Fleischhack, Ph. Levermann, Ashtekar variables: structures in bundles. e-print: 1112.1262 [math-ph]
34. Y. Fourès-Bruhat, Théorème d'existence pour certains systèmes d'équations aux dérivées partielles non linéaires. Acta Math. **88**, 141–225 (1952)
35. K. Giesel, Th. Thiemann, Algebraic quantum gravity (AQG) I. Conceptual setup. Class. Quantum Gravity **24**, 2465–2498 (2007)
36. D. Giulini, What is the geometry of superspace?. Phys. Rev. **D51**, 5630–5635 (1995)
37. M. Hanusch, A characterization of invariant connection. SIGMA **10**, 025 (2014)
38. M. Hanusch, Invariant connections and symmetry reduction in loop quantum gravity (Dissertation), Universität Paderborn (2014)
39. M. Hanusch, Invariant connections in loop quantum gravity, e-print: 1307.5303 [math-ph]
40. R.M. Hardt, Stratification of real analytic mappings and images. Invent. Math. **28**, 193–208 (1975)
41. J. Harnad, S. Shnider, L. Vinet, Group actions on principal bundles and invariance conditions for Gauge fields. J. Math. Phys. **21**, 2719–2724 (1980)
42. G. Immirzi, Real and complex connections for canonical gravity. Class. Quantum Gravity **14**, L177–L181 (1997)
43. R.C. Kirby, *The Topology of 4-Manifolds*. Lecture Notes in Mathematics, vol. 1374 (Springer, Berlin/Heidelberg, 1989)

44. J. Lewandowski, A. Okołów, H. Sahlmann, Th. Thiemann, Uniqueness of diffeomorphism invariant states on holonomy-flux algebras. Commun. Math. Phys. **267**, 703–733 (2006)
45. S. Łojasiewicz, Triangulation of semi-analytic sets. Ann. Scuola Norm. Sup. Pisa **18**, 449–474 (1964)
46. G.J. Murphy, *C^*-Algebras and Operator Theory* (Academic, San Diego, 1990)
47. A.D. Rendall, Comment on a paper of Ashtekar and Isham. Class. Quantum Gravity **10**, 605–608 (1993)
48. H. Ringström, *The Cauchy Problem in General Relativity*. ESI Lectures in Mathematics and Physics (European Mathematical Society, Zürich, 2009)
49. J. Samuel, Is Barbero's Hamiltonian formulation a Gauge theory? Class. Quantum Gravity **17**, L141–L148 (2000)
50. N. Straumann, *General Relativity: With Applications to Astrophysics* (Springer, Berlin/New York, 2004)
51. Th. Thiemann, Anomaly-free formulation of non-perturbative, four-dimensional Lorentzian quantum gravity. Phys. Lett. **B380**, 257–264 (1996)
52. Th. Thiemann, Quantum spin dynamics (QSD). Class. Quantum Gravity **15**, 839–873 (1998)
53. Th. Thiemann, *Modern Canonical Quantum General Relativity*. Cambridge Monographs on Mathematical Physics (Cambridge University Press, Cambridge, 2007)
54. R.M. Wald, *General Relativity* (Chicago University Press, Chicago, 1984)
55. H. Wang, On invariant connections over a principal fibre bundle. Nagoya Math. J. **13**, 1–19 (1958)
56. J.A. Zapata, A Combinatorial approach to diffeomorphism invariant quantum gauge theories. J. Math. Phys. **38**, 5663–5681 (1997)

Cosmic Puzzles: Dark Matter and Dark Energy

Gerhard Börner

Contents

Abstract In cosmology the peculiar situation arises that all the parameters of a standard cosmological model are precisely measured, whereas within the context of this model 95 % of the cosmic matter and energy density are unknown quantities: 27 % are accounted for by nonbaryonic dark matter particles, and 68 % by a mysterious something called dark energy. The astronomical observations leading to this conclusion are presented in this article, the status of the experiments searching for dark matter is reviewed, and some aspects of possible connections between dark energy and fundamental theories are discussed.

G. Börner (✉)
Max-Planck-Institute for Astrophysics, Karl-Schwarzschild-Str. 1, 85748 Garching, Germany
e-mail: grb@mpa-garching.mpg.de

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_12

Keywords Cosmology • Dark matter • Dark energy • Friedmann-Lemaître models • Cosmological constant • Type Ia supernova • Cosmic microwave background • Alternative theories of gravity

1 Introduction and Outline

Over the past 15 years, the global properties of the universe have been well-determined by astronomical observations. The term "universe" should just be understood as the system of galaxies accessible to us. In that system, supernovae of type Ia (SNe Ia) have been identified as reliable distance indicators, allowing to measure the cosmic expansion to a precision of a few percent (cf. Sect. 2). Quite surprisingly, a small deviation from the linear Hubble relation

$$cz = H_0 d, \tag{1}$$

where z is the redshift, d the distance, H_0 the Hubble constant, and c the speed of light, was detected, indicating that the expansion is accelerating. Detailed studies of galaxies and clusters have revealed the existence of dark matter. These results are in full agreement with the determination of cosmic parameters from the analysis of anisotropies in the cosmic microwave background (CMB).

It turns out that simple Friedmann-Lemaître (FL) cosmological models can accommodate all the data. These models are derived from Einstein's theory of General Relativity (GR), and they describe the evolution of a homogeneous and isotropic fluid in a curved spacetime characterized by pressure p and density ρ which are functions of time only (for the basic description of cosmology, I recommend two textbooks [1, 2]). This can only be an approximation to the present state of the universe, if the matter and radiation content is smoothed out over large scales, but it seems to be adequate to derive global properties. Especially for early phases, when density contrasts are small, the approximation becomes better.

The following rough picture emerges: the expansion time, the inverse of the Hubble constant H_0, is about 14 billion years. The total density is about equal to the critical density, defined as

$$\rho_c = \frac{3H_0^2}{8\pi G}, \tag{2}$$

where G is the gravitational constant. Only a small fraction of the density of about 5 % is contributed by the baryonic matter, the "normal" matter consisting of protons, neutrons, and electrons. About 27 % must be attributed to dark matter, clumps of nonbaryonic particles. All this adds up to 32 %, leaving a deficit in the balance of 68 %, something which is distributed uniformly in space. Many call this "dark energy", not a very appropriate name, because we know since Einstein that matter and energy are essentially the same. "Dark" matter and "dark" energy are, however,

very different: Whereas the mass in a comoving volume stays constant, the amount of dark energy in a comoving volume increases with the volume. This stuff seems to behave like a tension of empty space, relentlessly driving the expansion. "Dark energy" is a name which hints at some mysterious substance, but pragmatically speaking there is no mystery, it is just another parameter introduced so that the model can fit the data better (compare [14]).

Albert Einstein had introduced a "cosmological constant" to describe the world model favored around 1915. Most astronomers at that time were convinced that the world was nothing but a uniform, infinite, unchanging assembly of stars. The attractive force of gravity would pull all the stars together into one big clump, if it were not balanced by a kind of repulsive gravity. A suitably chosen constant in the equations can provide that balance (see Sect. 2). This approach fell into disrepute, of course, once the expansion of the system of galaxies was discovered by Edwin Hubble in the years after 1920. Moreover, this model is unstable against small perturbations which drive it into expansion or collapse.

Now, astronomers have reinstalled the cosmological constant by recent very precise measurements of the Hubble expansion. The data show that a cosmological constant must account for about 68 % of the total energy content. This contribution does not necessarily have to be just a constant. It might be a kind of potential energy of a scalar field which could perhaps change with time, although it looks like a cosmological constant now. There are as yet no convincing theoretical explanations for the dark energy, but the attempts to understand it from a fundamental physics point of view are vigorously pursued. Here seems to be an edge, where cosmology and fundamental physical theories meet. The astronomical observations are supported and confirmed by the analysis of the anisotropies of the CMB. From the power spectrum of the temperature fluctuations in the CMB sky, all the cosmic parameters can be determined (see Sect. 2). This is an independent piece of evidence, and the fact that what is measured from the CMB agrees with the observations made from stars and galaxies, indicates that the universe around us is well described by a simple FL model with all its parameters precisely determined.

In what follows, I will first (Sect. 2) discuss in some detail the astronomical observations, and how they can all be nicely accommodated by a cosmological model. This is the big success of modern cosmology. It works only, when dark matter and dark energy are included in the picture. Therefore, I will describe in Sects. 3 and 4 what we know of these two components of the cosmic substrate at present. Possible connections to fundamental physics will be pointed out, and finally the open questions remaining will be emphasized.

2 Measuring the Universe

The big telescopes have revealed a cosmos of galaxies of a great variety in shape and luminosity (see Fig. 1, a famous sky map obtained with the Hubble Space Telescope).

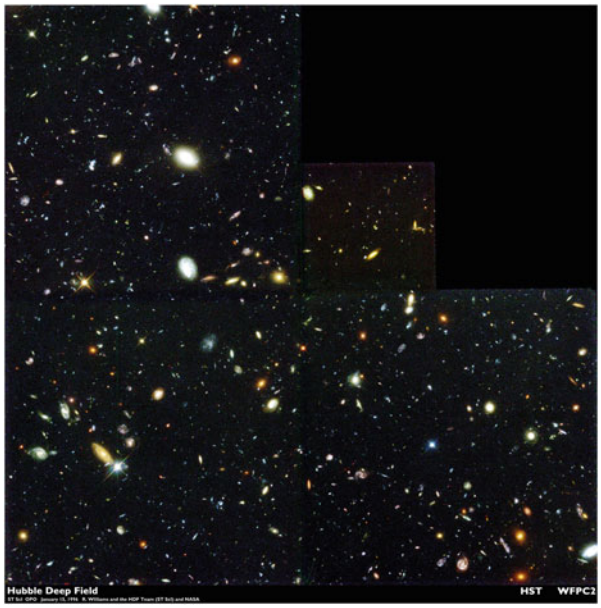


Fig. 1 The Hubble Deep Field is one of mankind's most distant optical views of the universe. The dimmest galaxies in this picture are as faint as 30th magnitude. This 1 arcmin by 1 arcmin field in URSA Major contains about 2500 galaxies. The Hubble Space Telescope was pointed at this single spot for 10 days (Courtesy of R. Williams, HDF team (Space Telescope Science Institute))

Two global properties of this system of galaxies are especially important: The spectral lines of each of these galaxies are shifted toward the red, i.e. toward the longer wavelengths. A few nearby galaxies, such as Andromeda, show a shift toward the blue. But for the majority the "redshift" can serve as a measure for the distance, as the American astronomer Edwin P. Hubble found in the 1920s. The further away a galaxy is, the larger is its redshift. Hubble found that redshift z and distance d are proportional to each other (cf. (1)). This rule holds for small values of z, i.e. moderate distances. It can be interpreted as a Doppler effect: The galaxies move away from us, and therefore the light emitted shows a Doppler-shift. Hubble's discovery changed the view of the cosmos dramatically. The idea of a static space filled uniformly with stars had to be given up. It was replaced by the picture of an expanding universe, where the galaxies move away from each other.

A second important point is just the fact that the velocity of light is finite. We cannot see distant cosmic objects as they are now, because the light emitted by them takes millions or billions of years to reach us. Astronomers see a kind of historical cross section of the cosmos, where distant objects also are far back in the past. If we follow the system of expanding galaxies back in time, we find that 14 billion years ago everything must have been very close together. The CMB, the cosmic radiation field, must have had a higher temperature at earlier epochs. This certainly is true as long as quantum gravity effects are not important, i.e. at thermal energies

below the Planck energy of 10^{19} GeV. Thus, it seems to be a safe conclusion that there must have been an extremely hot and dense early phase of the universe. All the galaxies and stars which we observe now could not have existed in that hot "big bang". According to the known laws of physics, they were dissolved in a structureless hot mixture of radiation and matter. The CMB gives us a record of the very early time, when this cosmic primeval soup became transparent. These are plausible considerations, and they can be made more quantitative in the framework of a theoretical cosmological model.

2.1 Friedmann-Lemaître Cosmological Models

For an isotropic and homogeneous space-time, the line element can be written in the form (see [1, 2])

$$ds^2 = -dt^2 + a^2(t)d\sigma^2 \tag{3}$$

with the velocity of light c set equal to 1. Here, t is the cosmic time which can be defined as the proper time of the matter, and $d\sigma^2$ is the line element of a 3-dimensional space of constant curvature. Physical distances between space-points at the same time t change proportional to an expansion factor $a(t)$. Inserting the metric given by (3) into the Einstein equations leads to two independent equations

$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi G}{3}\rho + \frac{\Lambda}{3} - \frac{\kappa}{a^2} \tag{4}$$

$$\ddot{a} = -\frac{4\pi G}{3}(\rho + 3p)a + \frac{1}{3}a\Lambda, \tag{5}$$

implying a kind of energy conservation:

$$\dot{\rho} = -3\left(\frac{\dot{a}}{a}\right)(\rho + p). \tag{6}$$

ρ and p are the density and pressure of the cosmic substrate, Λ is the cosmological constant, and κ the normalized curvature equal to 0 or $\pm$ 1; time derivatives d/dt are written by a dot. If p is nonzero, an equation of state $p(\rho)$ must be given to determine the solutions of (4) and (5).

The particles of the fluid characterized by $\rho(t)$, $p(t)$ are separation increases with time proportional to $a(t)$, and at the present time t_0, the rate $(\dot{a}/a)(t_0)$ is the Hubble constant H_0. For $p = 0$, we find from (6) that ρa^3 is constant in time – the mass in a comoving volume is conserved. If we take Eq. (4) at the present time, divide by H_0^2,

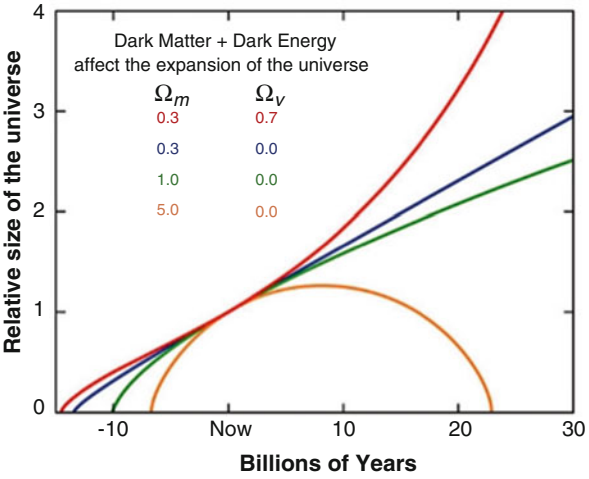


Fig. 2 The qualitative time evolution of the expansion factor of FL cosmological models (here plotted as "Relative size of the Universe" vs. Time) is shown in its dependence on the energy density Ω_m and Ω_V, where the latter symbol corresponds to Ω_Λ in the text. All models start from an initial singularity, where the expansion factor is zero, and as a consequence density and curvature become infinite. This singular beginning marks the breakdown of the classical models. Probably quantum gravity eventually will give an improved description of the models close to the singular beginning. The model with $\Omega_m = 0.3$, $\Omega_V = 0.7$ is favored by observations. The *orange graph* is for an unrealistic model with $\Omega_m = 5.0$ and $\Omega_V = 0.0$ which shows a maximum expansion and at late times a recollapse

we find

$$\Omega_m + \Omega_\Lambda + \Omega_\kappa = 1,$$

where we have used the conventions

$$\Omega_m = \frac{\rho(t_0)}{\rho_c}, \quad \Omega_\Lambda = \frac{\Lambda}{3H_0^2}, \quad \Omega_\kappa = -\frac{\kappa}{a_0^2 H_0^2}$$

with the critical density ρ_c given in (2). We can also derive the relation

$$\frac{\ddot{a}_0}{a_0 H_0^2} = \Omega_\Lambda - \frac{\Omega_m}{2}.$$

If $\Omega_m/2$ is greater than Ω_Λ, the expansion is decelerated, if Ω_Λ is greater than $\Omega_m/2$ the expansion accelerates. In Fig. 2, the graph of $a(t)$ is plotted for different sets of parameters. The static solution originally favored by Einstein is determined by

$$\Lambda = a^{-2} = 4\pi G\rho \qquad \text{and} \qquad \kappa = +1.$$

The different solutions shown in Fig. 2 correspond to possible different mixtures of matter, radiation, and eventually other types of energy. Each one of these components can be written as a fraction of the critical density. We may also incorporate Λ into the energy-momentum tensor of the cosmic substrate, and with $\Lambda = 8\pi G\rho_\Lambda$ and $p_\Lambda = -\rho_\Lambda$, consider $\rho + \rho_\Lambda$ and $p + p_\Lambda$ as generalized density and pressure. Then (4) becomes

$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi G}{3}\rho - \frac{\kappa}{a^2} \tag{7}$$

and (5)

$$\ddot{a} = -\frac{4\pi G}{3}(\rho + p). \tag{8}$$

In this form, the interpretation of Λ as a kind of vacuum energy seems quite natural. GR describes the geometry and quantum field theory gives the "vacuum energy". There are problems, however: "vacuum energies" derived from known field theories are too large, and lead to discrepancies with cosmological observations. Very likely a quantum description of the geometry must be found in order to arrive at a consistent picture. More about this in Sect. 4.

2.2 The Hubble Diagram of SNe Ia at High Redshifts

Naively, one plots a Hubble diagram as a graph where the velocities of galaxies are plotted versus distance. For objects at cosmic distances, however, neither distance nor velocity are directly measurable quantities. One commonly uses a formally defined luminosity distance D_L

$$D_L = \left(\frac{L}{4\pi F}\right)^{1/2}, \tag{9}$$

where L is the intrinsic luminosity of the source and F is the observed flux of energy. It is convenient to set D_L proportional to the "Hubble radius" c/H_0, and define a dimensionless quantity d_L:

$$D_L = \frac{c}{H_0} d_L. \tag{10}$$

In all FL models, d_L is a function of the redshift z and the important cosmic parameters Ω_m and Ω_Λ, where Ω_m includes all types of matter, also any kind of dark matter. Plotting $d_L(z; \Omega_m, \Omega_\Lambda)$ versus z gives a Hubble diagram. Astronomers commonly use logarithmic forms for L and F, so-called absolute and apparent

magnitudes M and m. The convention is to define the difference $m - M$ (the so-called distance modulus) such that

$$m - M \simeq 5\,log(D_L/1\,\mathrm{Mpc}) + 25,$$

or equivalently

$$m = \mu + 5\,log\big(d_L(z;\Omega_m,\Omega_\Lambda)\big) \tag{11}$$

with

$$\mu = M - 5\,log(H_0 \times 1\,\mathrm{Mpc}/c) + 25$$

(Mpc = Megaparsec: 1 Mpc $\simeq$ 3.28 million light years). Standard candles are objects which ideally have constant absolute magnitude M, and thus μ is a constant. A relation between m and z determined from observations will give constraints on Ω_m and Ω_Λ. The main task is to find suitable standard candles, and it has turned out that SNe Ia are very promising candidates. The spectrum of these exploding stars does not contain any hydrogen lines, only spectral lines of heavier elements like helium, carbon, or oxygen. Very likely these are white dwarfs – compact stars with the radius of the earth and the mass of the sun. The white dwarf star probably is in orbit around a companion in a narrow binary system. Mass flows from the companion to the white dwarf, it grows in mass until it reaches the critical Chandrasekhar mass, and becomes unstable. Then the gravitational collapse to a neutron star occurs, or the degenerate carbon interior ignites, and a subsonic nuclear burning front propagates outwards, and tears the white dwarf apart. In a few seconds the stellar material is transformed into Ni^{56} and other elements between Si and Fe. Ni^{56} decays into Co^{56} and later into Fe^{56}. This radioactive decay produces the luminosity of the supernova. SNe Ia are very bright and can be seen in far away galaxies. They light up within a few hours or a few days, and then decay in the course of several weeks.

Astronomers have found an empirical relation which allows them to determine the maximum luminosity of a supernova from the shape of the lightcurve. A slow decline of the lightcurve means that the peak luminosity is greater, while a fast decline is usually connected with a smaller maximum. The quantitative determination of this relation requires a calibration with supernovae whose distances are known (e.g. from a Cepheid measurement), and many detections of supernovae close to the maximum brightness. Over the years this has been achieved, such that cosmic distances can be measured now with an accuracy of better than 10 %. There remain, of course, systematic uncertainties which are difficult to take into account, especially the extinction of the radiation by intergalactic dust and evolutionary effects on the appearance of SNe Ia such as changes in progenitor mass, in the carbon to oxygen ratio over cosmic times. Theoretical models cannot yet predict the outcome of SNe Ia explosions reliably since the complex physics of these thermonuclear events requires multidimensional numerical simulations which must

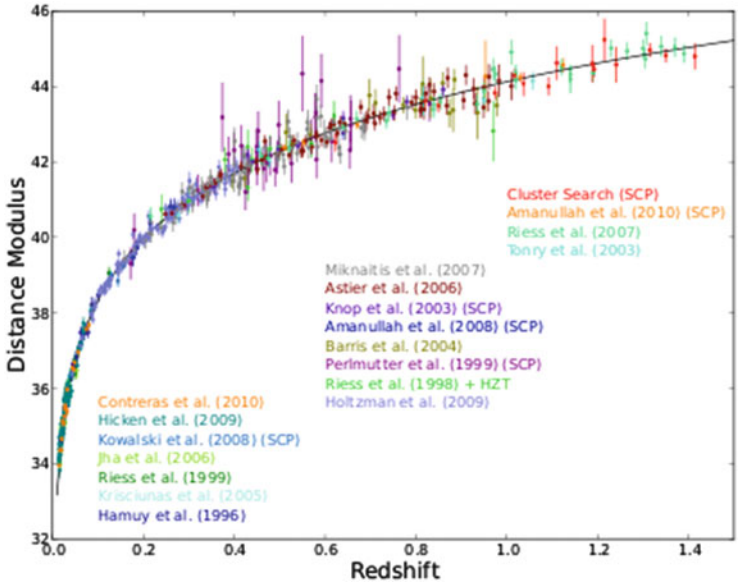


Fig. 3 Magnitude-redshift relation (Hubble-diagram) for a recent compilation of the data for 580 SNe (union 2.1 sample arXiv: 1105.3470). The drawn out line corresponds to the best fit model ($\Omega_\Lambda = 0.7, \Omega_{\text{tot.}} = 1$) [3] (Source: http://www.supernova.lbl.gov/Union)

include the treatment of strong turbulence. The studies accomplished so far show that quite a variation in the amount of Ni^{56} is likely, and hence a range of peak luminosities.

In view of these uncertainties, it is quite remarkable that the empirical relations allow to push the intrinsic dispersion in peak luminosities below $\Delta m = 0.17$. Figure 3 shows a Hubble diagram of 580 SNe [3], where the distance modulus μ is plotted against the redshift z. The line drawn through the data points corresponds to a cosmological model with total density $\Omega_{\text{tot.}} = 1$, matter density Ω_m about 0.3, and dark energy Ω_Λ about 0.7. The Hubble constant is found as $H_0 = 70$ in units of kilometers per second per Megaparsec. In Fig. 4, we can see how the supernova data can discriminate between different cosmological models [4]. The most surprising result of these measurements is that the distant supernovae are actually more distant than we would guess from Hubble's law (1). They must have been accelerated for some time in concordance with the acceleration ($\ddot{a} > 0$) caused by a positive cosmological constant.

This observational fact has led many to consider seriously a mysterious "dark energy" as the dominant component of the cosmic energy density, although it may be nothing else than a cosmological constant. This spectacular result has been confirmed by the analysis of the anisotropies of the CMB. The cosmic microwave radiation arrives almost isotropically in the wave length range between 0.5 mm and 10 cm, and its spectrum agrees perfectly with a theoretical Planck spectrum at a

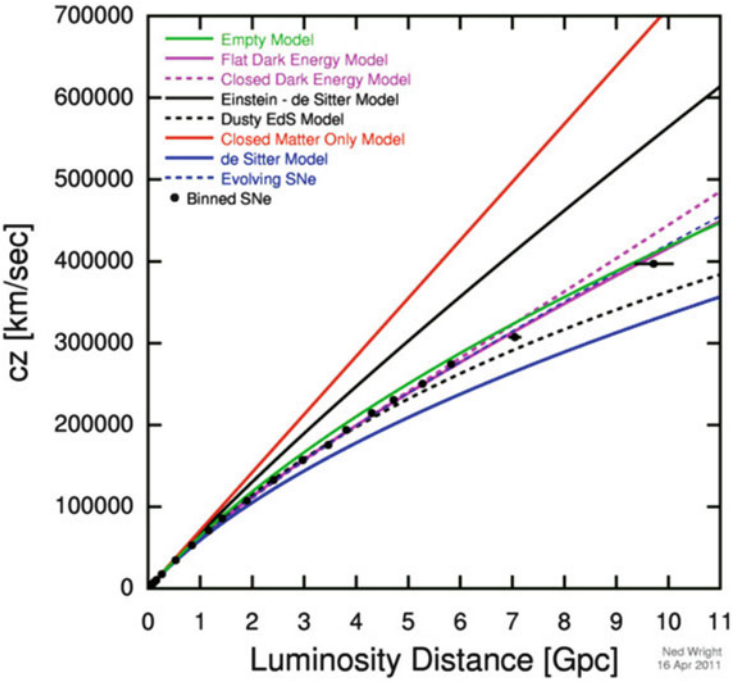


Fig. 4 Here, the differences in the magnitude-redshift relation for different cosmological models are shown. The supernova data can best be fitted by a model with $\Omega_\Lambda = 0.7, \Omega_{\text{tot.}} = 1$, the *magenta colored line* (Source: Legacy supernova survey (http://www.cfht.hawaii.edu/SNLS/) [4])

temperature of 2.728 K (Fig. 5) [5]. From Eq. (6), one finds for the energy density of a radiation field $\rho a^4 = \text{const.}$, and therefore the temperature T proportional to a^{-1}. Thus, the temperature decreases in proportion to the growth of the expansion factor, and at early times, it was correspondingly higher, eventually reaching thermal energies of the order of the Planck energy of 10^{19} GeV close to the big bang. As long as the temperature was above 3000 K, matter and radiation were in thermal equilibrium. Below that temperature, atoms could form, the free electrons became bound, and radiation and matter decoupled. This occurred at a redshift of about 1100, 380,000 years after the big bang.

An observer today detects the photons that had their last interaction with matter at a redshift of $z \simeq 1000$, a look at the cosmos before stars and galaxies existed. The CMB is almost smooth, but tiny variations in intensity across the sky of the order of 10^{-5} can be detected. Figure 6 shows the pattern of the angular temperature fluctuations on the celestial sphere, obtained from measurements of the PLANCK satellite. This figure is a snapshot of the distribution of radiation and energy at the moment of recombination, giving us a picture of the universe when it was a thousand times smaller and a hundred thousand times younger than today. In the PLANCK sky map, the features subtending a given angle are associated with physics on a

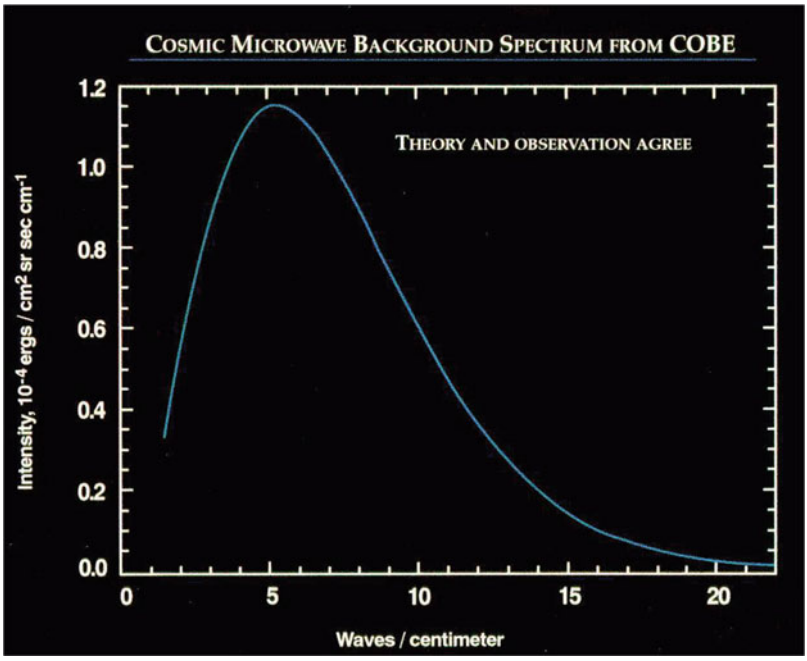


Fig. 5 The spectrum of the cosmic microwave radiation as it has been registered by the satellite COBE fits perfectly the formula for thermal radiation with a temperature of 2.728 K. Measurement uncertainties are less than 2 mK (± 0.002 K) (Source: COBE collaboration: [5])

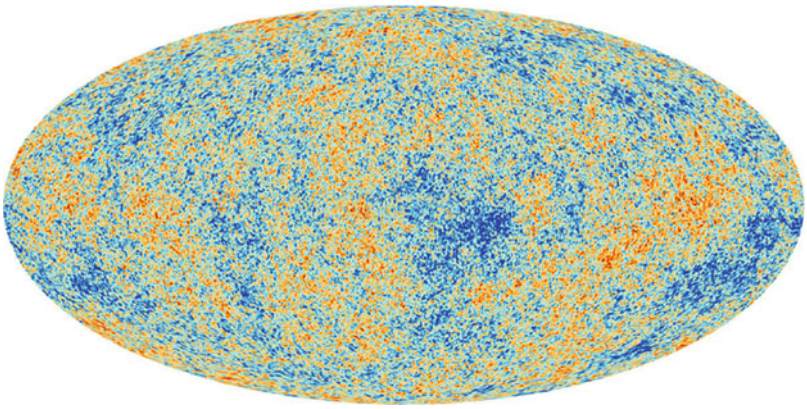


Fig. 6 A sky map of the CMB as obtained from the data of the PLANCK satellite shows hot (*red*) and cold (*blue*) spots in the temperature distribution with an amplitude of $\Delta T/T$ of order 10^{-5} (Source: ESA/PLANCK)

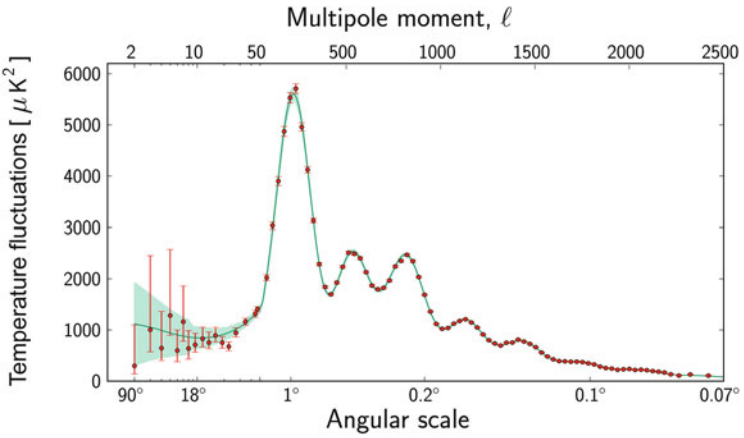


Fig. 7 The graph in this figure is the power spectrum of CMB anisotropies obtained from the PLANCK sky maps. It shows the square of the temperature fluctuations expanded in terms of multipoles. The location of the first maximum at $\ell \simeq 200$, or an angle $\simeq 1°$, shows that the spatial curvature of the cosmos is zero. The *solid curve* corresponds to a best- fit cosmological model (Source: ESA/PLANCK)

spatial scale that can be computed from the angle and the angular diameter distance to the last scattering surface. The latter depends on the cosmological model. The physical processes responsible for the pattern are closely connected to the formation of structures in the cosmos. Before recombination, small condensations in the dark matter distribution existed already, and the plasma of photons and baryons followed the gravitational pull of these condensations, but the radiation pressure of the photons worked against this. Thus, the plasma clouds started to oscillate. The largest cloud had been passed by such a pressure wave just once since recombination. Larger clouds could not build up pressure, but just followed gravity, and contracted slowly. Smaller clouds oscillated with a higher frequency. All oscillations were in phase, perfectly synchronized by the big bang. During the contraction of the cloud, the photon gas heated up, during expansion it cooled. At the recombination time, the photons left the plasma clouds with slightly different temperatures, and show up now as hot and cold spots on the CMB sky.

The statistical properties of these hot and cold regions of different angular size can be determined from an autocorrelation function of the temperature differences ΔT across the sky. This shows a sequence of clearly defined maxima (Fig. 7). The data points are derived from a multipole expansion of $(\Delta T)^2$ characterized by an index ℓ. Larger values of ℓ describe smaller angular scales. The angular scale around $\ell \simeq 200$ (corresponding to an angle of $\simeq 1°$) is the location of a prominent maximum. The physical scale corresponds roughly to the Hubble radius at recombination which is the dividing line between the large-scale inhomogeneities that have not changed much since their generation, and the small-scale perturbations which have become smaller than the horizon before recombination and have been

substantially modified by the action of gravity. The power spectrum shown in Fig. 7 gives us direct information about the primordial spectrum of perturbations for ℓ less than 200, and for $\ell > 200$ it enables us to derive all the parameters of the cosmological model with high precision [6]. For a thorough description of how this works, I recommend [2].

The latest results from the PLANCK satellite data tell us that the total density is equal to the critical density

$$\Omega_{\text{tot.}} = 1.$$

The matter component contributes 31.7 %, about 4.9 % are baryonic, 26.8 % are due to dark matter, as yet unknown. There remains a deficit of 68.3 % of some stuff which does not cluster on the scale of superclusters of galaxies. This has been given the name "dark energy". It is the same quantity found from the accelerated Hubble expansion, and it also agrees numerically. The accuracy of these measurements is a few percent.

3 Dark Matter

3.1 Candidates

The CMB data indicate that the cosmic matter amounts to about 32 % of the critical density, and that only 5 % of it is baryonic. This number is also obtained when one considers the synthesis of the lightest elements deuterium, helium, and lithium in the hot big bang, and compares theoretical results with astronomical measurements of the abundances of these elements. The baryons observed in stars, or as a diffuse gas producing X-rays, are only a fraction of this. So, even most of the baryonic matter is dark (see, e.g. [1, 2]). Twenty-seven percent of the matter is dark and non-baryonic, and as yet unknown. It is an experimental challenge to find out the nature of these particles. There are many particle physics candidates, and many experiments, but no evidence as yet.

Some constraints can be derived for these candidates from the cosmological model: They may have originated via decoupling from the thermodynamic equilibrium phase in the hot early universe, or they may have come from some nonthermal process. Thermal relics may be relativistic or nonrelativistic at the moment of decoupling. The relic particles which were relativistic at decoupling are called "hot dark matter", while "cold dark matter" is the name for the particles which were nonrelativistic at the decoupling time. The neutrino and the neutralino are examples of hot and cold relics, respectively.

In the beginning of dark matter research, a typical candidate for hot dark matter were neutrinos. They are the only kind of nonbaryonic dark matter known to us. It is known from the observation of solar neutrinos, and other experiments with neutrino oscillations, that they have a nonzero mass. The mass difference between

the electron neutrino and the μ- or τ- neutrino is typically

$$0 < (\Delta m)^2 \leq 10^{-4}(\mathrm{eV})^2.$$

If the neutrino masses are different, such that, e.g.

$$m_{\nu_e} < m_{\nu_\mu} < m_{\nu_\tau},$$

then their masses are also proportional to $\sqrt{(\Delta m)^2}$. Masses of the order of 10^{-2}eV may be a very realistic possibility. A degenerate mass spectrum, where the different types of neutrinos have almost equal masses with small mass differences may still be a possibility. Then the neutrino mass would be subject to an upper limit $m_\nu \leq 2.2$eV derived from β-decay experiments.

However, neutrinos cannot be the right candidate for dark matter particles for two reasons: They decouple when the temperature drops below 1 MeV, when only electrons, positrons, and photons are still in thermal equilibrium. For each neutrino species we have today

$$n_{\nu_0} = 109(T\gamma_0/2.7\,\mathrm{K})\,\mathrm{cm}^{-3}.$$

The density parameter is then

$$h_0^2\Omega_\nu = \rho_\nu/\rho_c = 0.01(T\gamma_0/2.7\,\mathrm{K})^3(m_\nu/1\mathrm{eV}),$$

where h_0 is the Hubble constant in units of $100\,\mathrm{km\,s^{-1}\,Mpc^{-1}}$. Then for the three types of neutrinos, we have with $h_0^2 \simeq 0.5$

$$\Omega_\nu \simeq 0.13 \qquad \text{in the case of mass degeneracy,}$$

$$\Omega_\nu \simeq 0.002 \qquad \text{in the most likely case of } m_\nu \simeq 10^{-2}\mathrm{eV}.$$

So, firstly, the neutrinos very likely do not contribute enough to the dark matter. Secondly, they are streaming with relativistic velocities when they decouple, and thus they damp out the inhomogeneities on scales smaller than the horizon scale at decoupling. This is a large scale $\simeq 13\Omega_\nu h_0^2(1+z)^{-1}$ Mpc, larger than the size of a galaxy cluster. As a result the large scale structure of the universe cannot be explained, because this certainly requires fluctuations on smaller scales. More promising are models, where cold relics constitute the dominant part of the dark matter. Cold relic particles decouple at temperatures corresponding to thermal energies much less than their rest mass energy. Therefore their number density n_x is exponentially suppressed in comparison with n_γ, the number density of photons. To estimate n_x at the time of decoupling, one equates their annihilation rate to the Hubble expansion rate

$$n_x < \sigma v >_{dec} \simeq H_{dec},$$

where $< \sigma v >_{dec}$ is the thermally averaged product of the annihilation cross section σ and the relative velocity v. With $x \equiv m_x/T_{dec}$, one finally obtains

$$\Omega_x h_0^2 \simeq g(T_{dec}) x^{3/2} \left(\frac{6 \times 10^{-38}\,\mathrm{cm}^2}{\sigma} \right). \tag{12}$$

Here, $g(T_{dec})$ is a statistical factor; see, e.g. [2]. Weakly interacting massive particles (WIMPs) which have masses between 10 GeV and a few TeV and cross sections of approximately electroweak strength $\sigma \simeq 10^{-38}\,\mathrm{cm}^2$ are ideal candidates for cold dark matter. Their number density freezes out at $x \sim 20$, and they may easily contribute the necessary 30 % to the total density of the universe. Several experiments have been set up to search for WIMPs. In the next section, a status report on these, up to now, unsuccessful searches is given.

3.2 Experimental Search for Dark Matter

The experiments to detect dark matter WIMPs directly via the interactions with ordinary matter on Earth are usually placed underground to reduce signal background caused by high-energy cosmic rays. A very sensitive experiment of this type is the Large Underground Xenon experiment (acronym LUX) at the Sanford Underground Laboratory in the Homestake Mine in South Dakota. LUX consists of an inner cryostat filled with 370 kg of liquid Xenon cooled to −100 °C. 122 photomultiplier tubes detect light generated inside the detector. A cylindrical water tank (8 m diameter, 6 m height) shields the detector from external radiation, such as gamma rays and neutrons. The underground depth of ∼1500 m provides shielding against cosmic rays. WIMPs interact exclusively with the liquid Xenon nuclei, resulting in nuclear recoils. These interactions produce photons and electrons which are registered. Neutron collisions with the Xe nuclei appear very similar. They must be minimized through shielding and the use of appropriate building material. Since WIMPs are so weakly interacting, most will pass through the detector unnoticed. WIMPs which interact will have a negligible chance of interacting again. Neutrons, on the other hand, have a reasonable large chance of multiple collisions within the target volume. Thus, one compares single interactions to multiple interactions, and once the ratio exceeds a certain value, the detection of dark matter is confirmed.

In Fig. 8, the results of measurements done in 2013 are shown [7]. The result is that so far there is no evidence for WIMP interactions. This is the most sensitive result so far, and it rules out low-mass WIMP signal hints from previous experiments. Below the blue line in Fig. 8 is the allowed range of cross section and WIMP mass. The whole upper region, where previous tentative claims for a detection are indicated, is excluded. Numerically the LUX experiment gives a minimum upper limit for the cross section $\sigma \leq 7.6 \times 10^{-46}\,\mathrm{cm}^2$ at a mass

$$m_{\mathrm{WIMP}} = 33\,\mathrm{GeV}/c^2$$

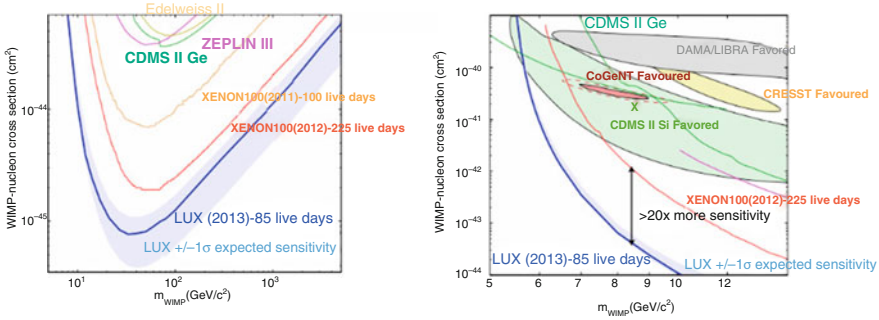


Fig. 8 The figure shows the 90 % confidence upper limit on the spin-independent WIMP-nucleon interaction cross section: LUX is compared to previous experiments. If WIMPs existed, as claimed by these earlier experiments, LUX should have seen about 1500 of them (Source: The LUX collaboration; [7]; http://www.lux.brown.edu)

(web-site: luxdarkmatter.org). The conclusion is clear: Up to now there is no detection of a dark matter particle. An upgrade of LUX is under construction. The experiments at the LHC in Geneva have detected the Higgs particle, but found no hint for physics beyond the standard model of elementary particles. Thus, there is also no indication which road should be followed when constructing theoretical extensions of the standard model.

3.3 Alternative Theories of Gravity

Maybe there is no dark matter after all? Maybe we are missing the point in postulating its existence, just as Ptolemy in ancient Egypt missed the point, when he introduced more and more epicycles to fit the motion of the celestial bodies to circles? This is the motivation behind the attempts to change the laws of gravity such that the observations can be explained without the need to introduce dark matter.

Modified Newtonian Dynamics (MOND; [8]) is the suggestion to set the Newtonian gravitational force not just equal to mass times acceleration, but to write

$$\vec{F}_N = m\mu\left(\frac{a}{a_0}\right)\vec{a}. \tag{13}$$

The acceleration $\vec{a}$ is multiplied by a function $\mu(a/a_0)$ with

$$\mu(x) \to \begin{cases} 1 & \text{for } x \gg 1 \\ x & \text{for } x \ll 1. \end{cases}$$

That is, for accelerations a small compared to a constant a_0, the force law is modified. Proponents of MOND typically choose something like

$$\mu(x) = (1 + x^{-2})^{-1/2}.$$

Then, for an object in circular orbit around a central mass M, one finds for a small acceleration $GM/r^2 = (1/a_0)(v^2/r)^2$, or

$$v^4 = GMa_0. \tag{14}$$

The velocity far away from the central mass is constant. More detailed fits to galactic rotation curves show that MOND can actually fit the observed rotation curves very well without the help of dark matter. The best fits are achieved for a value of the fundamental acceleration

$$a_0 = 1.2 \times 10^{-10}\,\mathrm{ms}^{-2}.$$

It is curious that MOND despite its ad hoc change of the dynamics can achieve good agreement with observations on the galactic scale. Still, MOND is so far just an alternative for Newtonian gravity. There is no underlying basic relativistic theory of gravitation for it, although some extensions of GR have been constructed which can lead to MOND type dynamics. These "Einstein-plus" theories consist of the addition of basic vector and scalar fields, contain additional parameters, but still cannot reproduce the full range of well-established results of GR (see, e.g. [10] for a review). Therefore, the majority of cosmologists stick to GR and the standard model of cosmology, and try to eventually solve the puzzles of dark matter and dark energy within this framework.

4 Dark Energy

4.1 Dark Energy Models

The existence of a positive cosmological constant is experimentally well established. From Fig. 9, we can clearly see how the combined evidence from CMB and supernova observations singles out a small region in the Ω_m-Ω_Λ plane. The region can be narrowed down more by including the now available measurements of baryonic acoustic oscillations, i.e. the signal recognizable in the clustering of structure in the universe today caused by the oscillations within the baryon-photon plasma before recombination. These measurements determine Λ, the second free constant in GR, and for the time being astronomers can be happy with that. No need to talk about a mysterious "dark energy". This pragmatic attitude is recommended, e.g. in [14]. But many cosmologists are not content with that: It is true that one

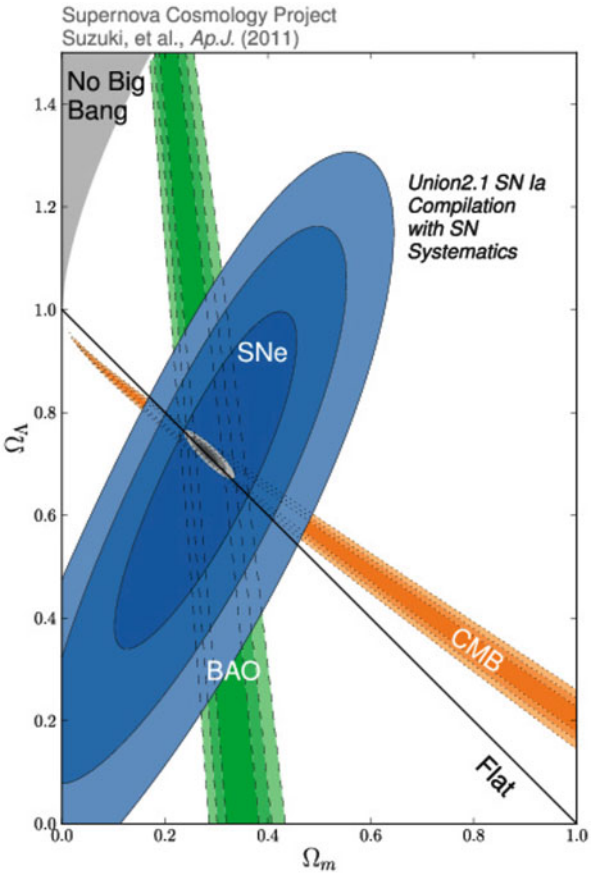


Fig. 9 68 %, 95 %, 99.7 % confidence limits obtained for Ω_m and Ω_Λ determinations from CMB (*orange*), Baryon Acoustic Oscillations (BAO, *green*), and the union 2.1 supernovae compilation (*blue*) are shown. The constraints allow a small range of values around $\Omega_\Lambda = 0.7, \Omega_m = 0.3$ (Source: http://www.supernova.lbl.gov/Union/; [3])

can view Λ just like Newton's constant G as experimental input to the theory, but it is curious that these two constants of nature are so different: G defines a huge energy scale, the Planck scale of $\sim 10^{19}\,\mathrm{GeV} = G^{-1/2}$, while the energy density $\Lambda/(8\pi G) = (10^{-12}\,\mathrm{GeV})^4$ is tiny compared to particle physics energies. We can phrase this in a different way: The cosmological constant defines a huge length scale $\Lambda^{-1/2}$ of about 10^{28} cm. Up to now nobody was able to bring this into contact with microphysical units of length.

Whether or not quantum physical effects can lead to an understanding is an open question at the moment. A deeper question is, why the typical ground state energy densities of quantum theories do not contribute gravitationally. This is a problem of quantum field theory, separate from the measured result of a positive Λ. Even for $\Lambda = 0$ this problem would be there [14]. In the following, I describe a few examples to illustrate the research activity in this field.

The first example is the interpretation of Ω_Λ as a dynamical quantity such as the energy density of a slightly time-varying scalar field. This case is referred to as

"quintessence". When we write the dark energy equation of state as

$$p = w\rho,$$

then $w = -1$ corresponds to a cosmological constant or a vacuum energy density. Any deviation of w from the value -1 points to a dynamical dark energy. It is a challenge for the observers to narrow the uncertainties. Up to now $w = -1$ is preferred. This would also have interesting consequences for the long-term future of the universe. If dark energy is a cosmological constant, then the acceleration of the expansion will continue forever, and the universe will become empty. If dark energy is caused by a dynamical scalar field, then this field may decay, and fill the universe again with matter and energy. The "quintessence" model [9] makes use of a scalar field with a tailor-made potential. The basic idea is that the cosmological constant is small because the universe is old. One considers a uniform scalar field with potential $V(\phi)$, and postulates a value ϕ_0 such that $dV/d\phi = 0$ at ϕ_0. The scalar field ϕ should approach this value, stay close to it, and change only slowly with time. The densities of matter and energy are steadily decreasing as the cosmos evolves, and eventually the potential energy dominates. Then the universe starts an exponential expansion with the expansion factor $a \sim exp(Ht)$, and

$$H^2(t) \simeq \frac{8\pi G}{3} V(\phi). \tag{15}$$

The problem is, of course, why $V(\phi)$ should be small and of the order of the present matter density at ϕ_0. It can be set up that way, if the potential is chosen appropriately. One can construct "tracker" solutions, where the cross-over from an early matter dominated expansion to a ϕ-field dominated expansion can be arranged such that the cross-over occurs just after recombination, and the desired properties arise. The task remains to imbed such a scalar field construction into a fundamental theory of particle physics. Scalar fields with the desirable effective potential just may not exist in such theories.

My second example is the model of inflationary cosmology [2]. The idea that a short phase of rapid, exponential expansion, much faster than the $a \simeq t^{1/2}$ law in the radiation dominated phase of the standard model, occurs in the early universe, has gained wide popularity. It seemingly explains various features of the standard model in a natural way: the high entropy, the very nearly zero spatial curvature, or equivalently the nearly critical energy density. The spectrum of initial density fluctuations can be calculated in inflationary models, and it agrees well with the measurements from the CMB. These are strong points in favor of an early stage of inflation. A scenario of this type almost appears to be necessary, because the horizon structure of the standard FL models without inflation would not allow a physically reasonable generation of density perturbations. It is an appealing scenario, but its foundations in a fundamental theory are not laid out convincingly yet. Most models employ a scalar field ϕ with potential energy $V(\phi)$. This looks very similar to the quintessence models, but so far a relation between the two types of models has

not been established. How can the large potential energy of the inflation field be thermalized almost completely, except for a tiny remainder? This is difficult to achieve in a natural way.

A third example, completely within classical physics, is that the back reaction of density inhomogeneities on the expansion may produce the measured effect of an accelerated cosmic expansion [13]. Unfortunately the back-reaction term has not been computed yet for a generic cosmological model, and one may suspect that it turns out to be just a negligible correction. Density inhomogeneities on the scale of galaxies and clusters are large, but the fluctuations of the gravitational potential are small, of order 0.01.

A fourth class of models for dark energy postulates deviations from GR. A critical review of the rapidly growing literature in this case is [10]. Generally, the alternative gravity models, such as the so-called $f(R)$ gravity (obtained by replacing the Einstein action $R - 2\Lambda$ by a function $f(R)$ of the Ricci scalar R) gain additional freedoms by slight extensions of GR. Such additional terms to the Einstein action are expected to arise from quantum gravity models. To explain dark energy, however, these $f(R)$ models need extreme fine tuning, and they all have severe problems of their own in addition.

4.2 Vacuum Energy and Dark Energy

Quantum theory does not know empty space. The vacuum is a complex state with fluctuating quantum fields and condensates of various kinds. For a space-time metric $g_{\mu\nu}$, we expect, because of Lorentz invariance, the vacuum expectation value of the energy momentum tensor to read

$$< T_{\mu\nu} >_{vac} = -g_{\mu\nu}\rho_{vac} + \text{higher order curvature terms.}$$

This would give rise to an effective cosmological constant $\Lambda = 8\pi G\rho_{vac} + \Lambda_0$, where Λ_0 is the bare cosmological constant in Einstein's field equations. Formally, however, ρ_{vac} is infinite, because it involves products of field operators at the same space-time point. Therefore, it has to be regularized and renormalized. In this context the energy density of the vacuum is rather an input to the renormalization than a prediction of the theory. It seems nevertheless reasonable to assume that the regularization is provided by the short distance behavior of the products of field operators. Then a natural choice for the regularization is a cutoff at the energy scale, where new physics is expected to appear. If one takes the Planck mass as the cutoff scale, one finds a ratio of $(10^{19}\,\text{GeV})^4$ to $(10^{-12}\,\text{GeV})^4$, i.e. a factor of 10^{123} over the value of the measured dark energy. Similarly at the GUT scale a factor of 10^{108}, and at the electro-weak scale of 1 TeV a factor of 2×10^{59} between the vacuum energy and the astronomical measurement of the cosmological constant. This is certainly a fantastic failure of a theoretical prediction. This huge discrepancy means that the vacuum energy densities must not be active gravitationally. An extremely precise

cancellation between the bare Λ_0 and $g_{\mu\nu}\rho_{vac}$ is required. At the moment there is no good theoretical idea which tells us how to achieve this.

Clearly this problem would exist, even if the cosmological constant was zero. But in some sense zero is not like any other number, because one might hope that some symmetry principle could be found which would set the contribution of vacuum energies exactly to zero and keep it at that value. A supersymmetric field theory may be a candidate, but such symmetries must be broken, since the real world is not supersymmetric. The breaking scale must be at least about 1 TeV, and thus the discrepancy remains huge. It seems difficult to derive a small, but nonzero number from a fundamental theory. Perhaps we have to wait for a theory of quantum gravity to illuminate this question.

Superstring theory has had an interesting connection with the cosmological constant [11]. First versions of superstring theory in ten dimensions gave rise to a negative or zero cosmological constant, and for some time it seemed as if the astronomical observations put the fundamental theory in trouble. Then it was discovered in the attempts to solve the "moduli problem", i.e. roughly speaking the problem of how to make the higher extra dimensions stable, that the set of 6-dimensional Calabi-Yau spaces occurring in the compactification of the theory to a four-dimensional manifold had a much richer structure than anticipated. It could be shown that in more complicated topologies the cosmological constant could acquire a small positive value. This was a great relief, but there was also a strange consequence to swallow: the number of independent classical background configurations found in this approach increased tremendously. One estimates that at least $\sim 10^{500}$ different solutions exist, each one giving rise to a different universe. The hope that a unique theory of strings could be found, seems to fade away. Instead a "landscape of superstring vacua", and a "landscape of different universes" has been proclaimed. In an act of desperation, so it seems, even famous physicists have voiced the view that we live in a "multiverse", and the properties of our universe can only be understood by the appeal to an "anthropic principle" [12]. This expresses the (trivial?) fact that we, perhaps generally intelligent life, can only exist in a world with specific properties. This argument is merely a logical consistency which might be regarded as a physical principle, if all these other worlds really existed. No one knows, and no one even knows, whether our real world is among the 10^{500} configurations of string theory. Maybe they are all unstable, and then we would be back at the pre-string theory status without a fundamental theory. Then it would not be the "end of physics", but a new beginning.

5 Outlook

It is fair to say that as of this time (mid-2015) there does not exist an explanation of dark energy from a fundamental physics. A nasty-minded person might add that many "models" are just a reformulation of the observational facts in the language of field theory. Seeing that there are many problems still unsolved should not give rise

to pessimism. Rather an optimistic outlook is appropriate: There is a lot to discuss, and the chances are great that we will understand more and more things about our world.

The most interesting aspect of the puzzles of dark matter and dark energy is in my opinion that in both cases experiments and observations are in principle capable of solving some of the problems: Within the next few years, one of the dark matter searches will very likely come up with a positive result. The equation of state of dark energy will be more precisely determined, and we will see whether a value of w different from -1 is found.

Of course, many theoretical problems remain. The strange composition of the cosmic substratum of 5 % baryonic matter, 27 % dark matter, and 68 % dark energy must be explained by some fundamental theory. Why do these values add up to the critical density? Why do we have dark matter and dark energy at all? Why do the energy densities present in our modern quantum field theories like QED or QCD not have any gravitational effect? Maybe we will have to wait for an answer until a unification of GR and quantum theory has been found.

Another good problem for theorists is connected to the idea of cosmic inflation. Why should the potential energy of the inflation field have huge gravitational effects in the early universe, leading to a rapid exponential expansion, while the vacuum energies of quantum field theories must not have any gravitational effect? An idea which makes this distinction plausible is certainly very desirable.

6 Web Sites

- Hubble Space Telescope – hubblesite.org – www.spacetelescope.org
- Supernova Projects – supernova.lbl.gov/Union – cf ht.hawaii.edu/SNLS
- CMB – lambda.gsfc.nasa.gov – sci.esa.int/planck/
- Dark Matter – lux.brown.edu

References

1. G. Börner, *The Early Universe – Facts and Fiction*, 4th edn. (Springer, Berlin, 2004)
2. V. Mukhanov, *Physical Foundations of Cosmology* (Cambridge University Press, Cambridge/New York, 2005)
3. N. Suzuki et al., The supernova cosmology project. Astrophys. J. **746**, 85 (2012)
4. A. Conley et al., Supernova constraints and systematic uncertainties from the first 3 years of the supernova legacy survey. Astrophys. J. Supp. **192**, 1 (2011)
5. J.C. Mather et al., A preliminary measurement of the CMB spectrum by the COBE satellite. Astrophys. J. **354**, L37 (1990); D. Fixsen et al., The CMB spectrum from the full COBE FIRAS data set. Astrophys. J. **437**, 576 (1996)
6. Planck 2013 results, XVI. Cosmological parameters. Astron. Astrophys. **571**, A16 (2014)
7. D.S. Akerib et al., First results from the LUX dark matter experiment at the Sanford underground facility. Phys. Rev. Lett. **112**, 091303 (2014)

8. M. Milgrom, Dynamics with a non-standard inertia-acceleration relation: an alternative to dark matter. Ann. Phys. **229**, 384 (1994)
9. C. Wetterich, *Inflation, Quintessence, and the Origin of Mass* (2014). arXiv 1408.0156
10. N. Straumann, *Problems with Modified Theories of Gravity as Alternatives to Dark Energy* (2008). arXiv 0809.5148
11. L. Smolin, *The Trouble with Physics* (Houghton Mifflin, Boston, 2006)
12. S. Weinberg, *Living in the Multiverse* (2005). 2005 hep-th/0511037
13. T. Buchert, Dark energy from structure – a status report. Gen. Rel. Grav. **40**, 467 (2008)
14. E. Bianchi, C. Rovelli, *Why All These Prejudices Against a Constant?* (2010). arXiv 1002.3966

Radiation and Scattering in Non-relativistic Quantum Electrodynamics

Israel Michael Sigal

Contents

Supported by NSERC Grant No. NA7901

I.M. Sigal (✉)
Department of Mathematics, University of Toronto, 40 St. George Street, Bahen Centre, Toronto ON M5S 2E4, Canada
e-mail: im.sigal@utoronto.ca

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_13

Abstract The standard model of non-relativistic quantum electrodynamics describes non-relativistic quantum matter, such as atoms and molecules, (minimally) coupled to the quantized electromagnetic field. This model provides mathematically solid and physically reasonable foundations for a description of all physical processes arising from the interaction of matter and radiation. We review basic notions, results and techniques in the theory of radiation and scattering, specifically, Rayleigh scattering, within this model. We also describe some ideas entering the proofs. This review is an extended version of the talk given at the Conference "Quantum Mathematical Physics", Regensburg, September/October, 2014.

Keywords Quantum electrodynamics • Photons and electrons • Renormalization group • Quantum resonances • Spectral theory • Schrödinger operators • Ground state • Quantum dynamics • Non-relativistic theory

Mathematics Subject Classification (2010). 81Q99, 81T10, 81T17, 81V10

1 Overview

The non-relativistic quantum electrodynamics (QED) was proposed in early days of Quantum Mechanics. It was already taken for granted in 1932 when Fermi ([37]) wrote his review of theory of radiation. It was elaborated in an important way in ([69]) and its rigorous analysis was pioneered in [38, 39]. It describes quantum-mechanical particle systems (minimally) coupled to the quantized electromagnetic field and arises from a standard quantization of a classical one (with possible addition of internal – spin – degrees of freedom). In fact, it is the most general quantum theory obtained as a quantization of a classical system. It gives a complete and consistent account of electrons and nuclei interacting with electro-magnetic radiation at low energies. It accounts for all physical phenomena in QED, apart from vacuum polarization. In particular, it deals successfully with renormalization of mass and energy and with the anomalous magnetic moment (see [7, 72, 79]). The main issues a QED theory has to address are

- Stability of elementary quantum systems such as atoms and molecules,
- Radiation,
- Scattering theory.

The headings above have the following translations into mathematical terms:

- Stability $\Longleftrightarrow$ Existence of the *ground state*,
- Radiation $\Longleftrightarrow$ Instability and decay of the excited states of particle systems,
- Scattering $\Longleftrightarrow$ Asymptotic behaviour of evolution at large times.

Remarkable progress was made in the last 10 or so years in constructing the rigorous theory of the stability, radiation and scattering. Three powerful and unifying techniques emerged as the result of this development: theory of *resonances*, giving a clear-cut mathematical description of processes of emission and absorption of the electro-magnetic radiation, the spectral *renormalization group*, giving the perturbation theory for bound states and resonances and the method of *propagation observables and propagation inequalities* underpinning the scattering theory.

In this brief review, we summarize progress on the first two items and give more details on the last one. In considering the long-time dynamics, we concentrate on energies below the ionization threshold (Rayleigh scattering). The review is based on the papers [35, 36]. We also borrow some general material from our previous review [73], to which we refer the reader for more details and references of the problems of stability and radiation (see also the review [4] and the book [79]).

We formulate the key problems related the long-time dynamics which is the area of concentration of this review. The Hamiltonian H of a non-relativistic particle system coupled to the quantized electromagnetic or phonon field is self-adjoint and generates the dynamics through the Schrödinger equation,

$$i\partial_t \psi_t = H\psi_t. \tag{1}$$

As initial conditions, ψ_0, we consider states below the ionization threshold Σ, i.e. ψ_0 in the range of the spectral projection $E_{(-\infty,\Sigma)}(H)$. In other words, we are interested in processes, like emission and absorption of radiation, or scattering of photons on a particle system (say, an atom or a molecule or an electron bound by an external potential) in which the particle system is not being ionized.

Denote by Φ_j and E_j the eigenfunctions and the corresponding eigenvalues of the Hamiltonian H, below Σ, i.e. $E_j < \Sigma$. The following are the key characteristics of the evolution of (1), in progressive order the depth of information they provide:

- *Local decay* stating that photons are either bound to the particle system or escape to infinity, i.e. the probability that they occupy any bounded region of the physical space tends to zero, as $t \to \infty$.
- *Minimal photon velocity bound* with speed c stating that, as $t \to \infty$, with the probability $\to 1$, the distance of the departing photons to the particle system $\geq c't$, for any $c' < c$.

  Similarly, if the probability that at least one photon is at the distance $\geq c''t$, $c'' > c$, from the particle system vanishes, as $t \to \infty$, we say that the evolution satisfies the *maximal photon velocity bound* with speed c.
- *Asymptotic completeness* on the interval $(-\infty, \Sigma)$ stating that, for any $\psi_0 \in \mathrm{Ran}\, E_{(-\infty,\Sigma)}(H)$, and any $\epsilon > 0$, there are photon wave functions $f_{j\epsilon} \in \mathcal{F}$, with a finite number of photons, s.t. the solution, $\psi_t = e^{-itH}\psi_0$, of the Schrödinger equation, (1), satisfies

$$\limsup_{t\to\infty} \left\| e^{-itH}\psi_0 - \sum_j e^{-iE_j t}\Phi_j \otimes_s e^{-iH_f t} f_{j\epsilon} \right\| \leq \epsilon. \tag{2}$$

(One can verify that $\Phi_j \otimes_s f_{j\epsilon}$ is well-defined, at least for the ground state ($j = 0$).) In other words, for any $\epsilon > 0$ and with probability $\geq 1 - \epsilon$, the Schrödinger evolution ψ_t approaches asymptotically a superposition of states in which the particle system with a photon cloud bound to it is in one of its bound states Φ_j, with additional photons (or possibly none) escaping to infinity with the velocity of light.

We give the rigorous definitions of the local decay, the photon velocity and asymptotic completeness in Appendix Appendix 5: and Sects. 4 and 5, respectively. The reason for $\epsilon > 0$ in (2) is that for the state $\Phi_j \otimes_s f_j$ to be well defined, as one would expect, one would have to have a very tight control on the number of photons in f_j, i.e. the number of photons escaping the particle system. (See the remark at the end of Subsection 5.4 of [35] for a more technical explanation.) For massive bosons $\epsilon > 0$ can be dropped (set to zero), as the number of photons can be bound by the energy cut-off.

The results and techniques discussed in this review are also applicable to the phonon Hamiltonians. The latter are discussed in Appendix Appendix 2:.

In order to make the review more accessible to non-experts, we included Supplement I defining and discussing the creation and annihilation operators (see also [24, 28]).

Notations For functions A and B, we will use the notation $A \lesssim B$ signifying that $A \leq CB$ for some absolute (numerical) constant $0 < C < \infty$. Furthermore, $D(A)$ denotes the domain of an operator A and $\langle x \rangle := (1 + |x|^2)^{1/2}$.

2 Schrödinger Equation

The *standard model of non-relativistic quantum electrodynamics* describes a non-relativistic quantum particle system minimally coupled to the quantized electromagnetic field. The state space for this model is given by $\mathcal{H} := \mathcal{H}_p \otimes \mathcal{F}$, where $\mathcal{H}_p$ is the particle state space, say, $L^2(\mathbb{R}^{3n})$, or a subspace thereof, and $\mathcal{F}$ is the bosonic Fock space, $\mathcal{F} \equiv \Gamma(\mathfrak{h}) := \mathbb{C} \oplus_{n=1}^{\infty} \otimes_s^n \mathfrak{h}$, based on the one-photon space $\mathfrak{h} := L^2(\mathbb{R}^3, \mathbb{C}^2)$ ($\otimes_s^n$ stands for the symmetrized tensor product of n factors, $\mathbb{C}^2$ accounts for the photon polarization). Its dynamics is generated by the Hamiltonian

$$H := \sum_{j=1}^{n} \frac{1}{2m_j} \big(-i\nabla_{x_j} - \kappa_j A_\xi(x_j) \big)^2 + U(x) + H_f. \tag{3}$$

Here, (a) m_j and x_j, $j = 1, \ldots, n$, are the ('bare') particle masses and the particle positions, $U(x)$, $x = (x_1, \ldots, x_n)$, is the total potential affecting the particles, and κ_j are coupling constants related to the particle charges, (b) $A_\xi := \check{\xi} * A$ is the *quantized vector potential* in the Coulomb gauge ($\operatorname{div} A(y) = 0$), subject to an *ultraviolet cut-off* ξ, satisfying e.g. $|\partial^m \xi(k)| \lesssim \langle k \rangle^{-3}$, and (c) H_f is the quantum Hamiltonian of the

quantized electromagnetic field. The operators A_ξ and H_f, describing the quantized electromagnetic field and its dynamics, respectively, are given by

$$A_\xi(y) = \sum_{\lambda=1,2} \int \frac{\xi(k)d^3k}{\sqrt{2\omega(k)}} \varepsilon_\lambda(k)\big(e^{ik\cdot y}a_\lambda(k) + e^{-ik\cdot y}a_\lambda^*(k)\big), \tag{4}$$

where, $\omega(k) = |k|$ denotes the photon dispersion relation (k is the photon wave vector), λ is the polarization, and $a_\lambda(k)$ and $a_\lambda^*(k)$ are photon annihilation and creation operators acting on the Fock space $\mathcal{F}$ (see Supplement II for the definition), and

$$H_f = \sum_{\lambda=1,2} \int d^3k\ \omega(k)a_\lambda^*(k)a_\lambda(k). \tag{5}$$

Here and in what follows, the integrals without indication of the domain of integration are taken over entire $\mathbb{R}^3$.

For simplicity we have omitted the interaction of the spin with magnetic field. (For a discussion of this Hamiltonian including units, the removal of the center-of-mass motion of the particle system and taking into account the spin of the particles, see Appendix Appendix 1:. Note that our units are not dimensionless. We use these units since we want to keep track of the particle masses. To pass to the dimensionless units we would have to set $m_{\text{el}} = 1$ also.)

We assume that $U(x) \in L^2_{\text{loc}}(\mathbb{R}^{3n})$ and is either confining or relatively bounded with relative bound 0 w.r.t. $-\Delta_x$, so that the particle Hamiltonian

$$H_p := -\sum_{j=1}^{n} \frac{1}{2m_j}\Delta_{x_j} + U(x),$$

and therefore the total Hamiltonian H, are self-adjoint. The Hamiltonian H determines the dynamics via the time-dependent Schrödinger equation

$$i\partial_t\psi = H\psi,$$

where ψ is a differentiable path in $\mathcal{H} = \mathcal{H}_p \otimes \mathcal{H}_f$.

A key fact here is that for the particle models discussed above, (both for the non-relativistic QED and phonon models), there is a spectral point $\Sigma \in \sigma(H) \cup \{\infty\}$, called the *ionization threshold*, s.t. below Σ, the particle system is well localized:

$$\|\langle p\rangle^2 e^{\delta|x|} f(H)\| \lesssim 1, \tag{6}$$

for any $0 \le \delta < \operatorname{dist}(\operatorname{supp} f, \Sigma)$ and any $f \in C_0^\infty((-\infty, \Sigma))$. In other words, states decay exponentially in the particle coordinates x ([7, 8, 50]). To guarantee that $\Sigma > \inf\sigma(H_p) \ge \inf\sigma(H)$, we assume that the potentials $U(x)$ or $V(x)$ are such that the particle Hamiltonian H_p has discrete eigenvalues below the

essential spectrum ([7, 8, 50]). Furthermore, Σ, for which (6) is true, is given by $\Sigma := \lim_{R\to\infty} \inf_{\varphi\in D_R}\langle\varphi, H\varphi\rangle$, where the infimum is taken over $D_R = \{\varphi \in \mathcal{D}(H)|\ \varphi(x) = 0 \text{ if } |x| < R, \|\varphi\| = 1\}$ (see [50]; Σ is close to $\inf\sigma_{\rm ess}(H_p)$).

2.1 Ultra-Violet Cut-Off

We reintroduce the Planck constant, $\hbar$, speed of light, c, and electron mass, $m_{\rm el}$, for a moment. Assuming the ultra-violet cut-off $\xi(k)$ decays on the scale k_0, in order to correctly describe the phenomena of interest, such as emission and absorption of electromagnetic radiation, i.e. for optical and rf modes, we have to assume that the cut-off energy,

$$\hbar c k_0 \gg \alpha^2 m_{\rm el}c^2, \text{ ionization energy, characteristic energy of the particle motion.}$$

On the other hand, we should exclude the energies where the relativistic effects, such as electron-positron pair creation, vacuum polarization and relativistic recoil, take place, and therefore we assume

$$\hbar c k_0 \ll m_{\rm el}c^2, \text{ the rest energy of the the electron.}$$

Combining the last two conditions we arrive at $\alpha^2 m_{\rm el}c/\hbar \ll k_0 \ll m_{\rm el}c/\hbar$, or in our units,

$$\alpha^2 m_{\rm el} \ll k_0 \ll m_{\rm el} \ .$$

The Hamiltonian (3) is obtained by the rescaling $x \to \alpha^{-1}x$ and $k \to \alpha^2 k$ of the original QED Hamiltonian (see Appendix Appendix 1:). After this rescaling, the new cut-off momentum scale, $k_0' = \alpha^{-2}k_0$, satisfies

$$m_{\rm el} \ll k_0' \ll \alpha^{-2}m_{\rm el},$$

which is easily accommodated by our estimates (e.g. we can have $k_0' = O(\alpha^{-1/3}m_{\rm el})$).

2.2 Generalized Pauli-Fierz Transformation

The coupling function $g_y^{\rm qed}(k,\lambda) := |k|^{-1/2}\xi(k)\varepsilon_\lambda(k)e^{ik\cdot y}$ in the QED Hamiltonian defined in (3) and (4) is more singular in the infrared than can be handled by our techniques. To go around this problem we use the (unitary) generalized Pauli–Fierz

transformation (see [72]) to pass to the new unitarily equivalent Hamiltonian

$$H \longrightarrow \tilde{H} := e^{-i\Phi(q_x)} H e^{i\Phi(q_x)}, \tag{7}$$

where $\Phi(h)$ is the operator-valued field, $\Phi(h) := \frac{1}{\sqrt{2}}(a^*(h)+a(h))$, and the function $q_x \equiv q_x(k,\lambda)$, where, recall, $x = (x_1, \ldots, x_n)$, is defined, for $0 < \nu < 1/2$, as

$$q_x := \sum_{j=1}^{n} \kappa_j \tilde{q}_{x_j}, \quad \text{with} \quad \tilde{q}_y(k,\lambda) := \frac{\xi(k)}{|k|^{\frac{1}{2}+\nu}} \varphi(|k|^\nu \varepsilon_\lambda(k)\cdot y). \tag{8}$$

Here $\varphi \in C^\infty(\mathbb{R};\mathbb{R})$ is a non-decreasing function such that $\varphi(r) = r$ if $|r| \leq 1/2$ and $|\varphi(r)| = 1$ if $|r| \geq 1$. We note that the definition of $\Phi(h)$ gives $A(y) = \Phi(g_y^{\text{qed}})$, where $g_y^{\text{qed}} := \frac{\xi(k)dk}{\sqrt{2|k|}} e^{ik\cdot y}$.

The Hamiltonian $\tilde{H}$ is of the same form as H. Indeed, using the commutator expansion $e^{-i\Phi(q_x)} H_f e^{i\Phi(q_x)} = -i[\Phi(q_x), H_f] - [\Phi(q_x), [\Phi(q_x), H_f]]$, we compute

$$\tilde{H} = \sum_{j=1}^{n} \frac{1}{2m_j} \big(-i\nabla_{x_j} - \kappa_j \tilde{A}(x_j) \big)^2 + E(x) + H_f + V(x), \tag{9}$$

where, recall, $x = (x_1, \ldots, x_n)$, and

$$\begin{cases} \tilde{A}(y) := \Phi(\tilde{g}_y), \quad \tilde{g}_y(k,\lambda) := g_y^{\text{qed}}(k,\lambda) - \nabla_x \tilde{q}_y(k,\lambda), \\ E(x) := -\sum_{j=1}^n \kappa_j \Phi(e_{x_j}), \quad e_y(k,\lambda) := i|k|\tilde{q}_y(k,\lambda), \\ V(x) := U(x) + \frac{1}{2}\sum_{\lambda=1,2}\sum_{j=1}^n \kappa_j^2 \int_{\mathbb{R}^3} |k||\tilde{q}_{x_j}(k,\lambda)|^2 dk. \end{cases} \tag{10}$$

The operator $\tilde{H}$ is self-adjoint with domain $D(\tilde{H}) = D(H) = D(p^2 + H_f)$ (see [54, 55]).

Now, the coupling functions (form factors) $\tilde{g}_y(k,\lambda)$ and $e_y(k,\lambda)$ in the transformed Hamiltonian, $\tilde{H}$, satisfy the estimates that are better behaved in the infrared ([11]):

$$|\partial_k^m \tilde{g}_y(k,\lambda)| \lesssim \langle k\rangle^{-3} |k|^{\frac{1}{2}-|m|} \langle y\rangle^{\frac{1}{\nu}+|m|}, \tag{11}$$

$$|\partial_k^m e_y(k,\lambda)| \lesssim \langle k\rangle^{-3} |k|^{\frac{1}{2}-|m|} \langle y\rangle^{1+|m|}. \tag{12}$$

We see that the coupling functions in the operator (9) have much better infrared behaviour, at least if one has a priori bounds controlling the large y behaviour. In proving the results discussed below, one first proves them for the generalized Pauli-Fierz Hamiltonian $\tilde{H}$ and then transfers the obtained information to the original Hamiltonian H.

3 Stability and Radiation

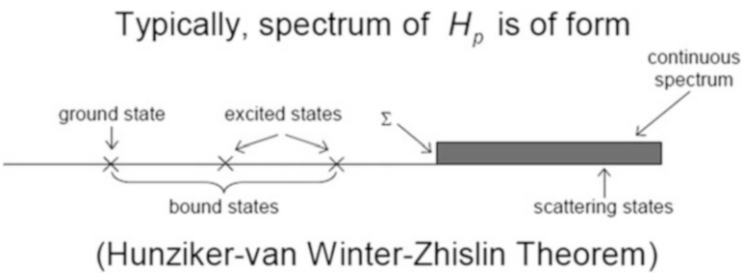
We assume for simplicity that our matter consists of electrons and the nuclei and that the nuclei are infinitely heavy and therefore are manifested through the interactions only (put differently, the molecules are treated in the Born – Oppenheimer approximation). In this case, the coupling constants κ_j are equal, $\kappa_j = \kappa$, related to the electron charge $-e$ as $\kappa := \alpha^{3/2}$, where $\alpha = \frac{e^2}{4\pi\hbar c} \approx \frac{1}{137}$, the fine-structure constant, and $m_j = m$. It is shown (see Sect. 7 and a review in [4] for references and discussion) that the physical electron mass, $m_{\rm el}$, is not the same as the parameter $m \equiv m_j$ (the 'bare' electron mass) entering (3), but depends on m and κ. Inverting this relation, we can think of m as a function of $m_{\rm el}$ and κ. If we fix the particle potential $U(x)$ (e.g. taking it to be the total Coulomb potential), and $m_{\rm el}$ and e, then the Hamiltonian (3) depends on one free parameter, the bare electron mass m (or the ultraviolet cut-off scale, κ).

3.1 Results

We begin with considering the matter system alone. As was mentioned above, its state space, $\mathcal{H}_p$, is either $L^2(\mathbb{R}^{3n})$ or a subspace of this space determined by a symmetry group of the particle system, and its Hamiltonian operator, H_p, acting on $\mathcal{H}_p$, is given by

$$H_p := \sum_{j=1}^{n} \frac{-1}{2m_j} \Delta_{x_j} + V(x), \tag{13}$$

where Δ_{x_j} is the Laplacian in the variable x_j and, recall, $U(x)$ is the total potential of the particle system. Under the conditions on the potentials $U(x)$, given above, the operator H_p is self-adjoint and bounded below. Typically, according to the HVZ theorem, its spectrum consists of isolated eigenvalues, $\epsilon_0^{(p)} < \epsilon_1^{(p)} < \ldots < \Sigma^{(p)}$, and continuum $[\Sigma^{(p)}, \infty)$, starting at the ionization threshold $\Sigma^{(p)}$, as shown in the figure below.



The eigenfunctions corresponding to the isolated eigenvalues are exponentially localized. Thus left on its own the particle system, either in its ground state or in one of the excited states, is stable and well localized in space. We expect that this picture changes dramatically when the total system (the universe) also includes the electromagnetic field, which at this level must be considered to be quantum. As was already indicated above what we expect is the following

- The stability of the system under consideration is equivalent to the statement of existence of the ground state of H, i.e. an eigenfunction with the smallest possible energy.
- The physical phenomenon of radiation is expressed mathematically as emergence of resonances out of excited states of a particle system due to coupling of this system to the quantum electro-magnetic field.

As a result, we would like to show that

(1) The *ground state* of the particle system is *stable* when the coupling is turned on, while
(2) The excited states, generically, are not. They turn into *resonances*.

3.2 Infrared Problem

The resonances arise from the eigenvalues of the non-interacting Hamiltonian $H_{\kappa=0}$. The latter is of the form

$$H_0 = H_{\text{part}} \otimes \mathbf{1}_f + \mathbf{1}_{\text{part}} \otimes H_f \,. \tag{14}$$

The low energy spectrum of the operator H_0 consists of branches $[\epsilon_i^{(p)}, \infty)$ of absolutely continuous spectrum and of the eigenvalues $\epsilon_i^{(p)}$'s, sitting at the continuous spectrum 'thresholds' $\epsilon_i^{(p)}$'s. Here, recall, $\epsilon_0^{(p)} < \epsilon_1^{(p)} < \ldots < \Sigma^{(p)}$ are the isolated eigenvalues of the particle Hamiltonian H_p. Let $\phi_i^{(p)}$ be the eigenfunctions of the particle system, while Ω be the photon vacuum. The eigenvalues $\epsilon_i^{(p)}$'s correspond to the eigenfunctions $\phi_i^{(p)} \otimes \Omega$ of H_0. The branches $[\epsilon_i^{(p)}, \infty)$ of absolutely continuous spectrum are associated with generalized eigenfunctions of the form $\phi_i^{(p)} \otimes g_\lambda$, where g_λ are the generalized eigenfunctions of H_f : $H_f g_\lambda = \lambda g_\lambda$, $0 < \lambda < \infty$.

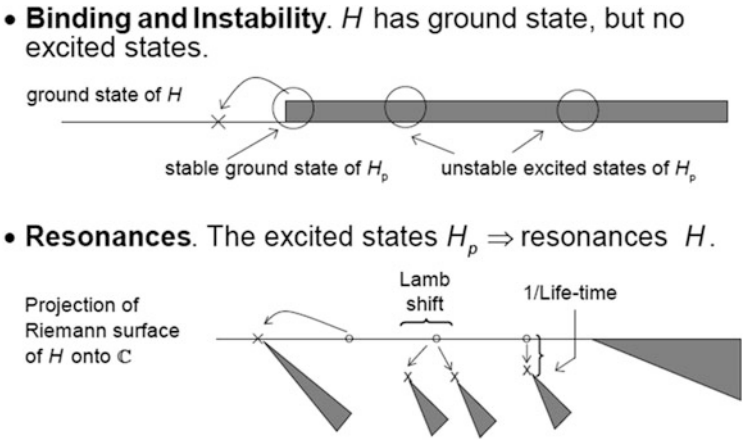
The absence of gaps between the eigenvalues and thresholds is a consequence of the fact that the photons are massless. To address this problem we use the spectral renormalization group (RG). The problem here is that the leading part of the perturbation in H is marginal.

3.3 Bifurcation of Eigenvalues and Resonances

Stated informally what we show is

- The ground state of $H|_{\kappa=0} \Rightarrow$ the ground state H ($\epsilon_0 = \epsilon_0^{(p)} + O(\kappa^2)$ and $\epsilon_0 < \epsilon_0^{(p)}$);
- The excited states of $H|_{\kappa=0} \Rightarrow$ (generically) the resonances of H ($\epsilon_{j,\kappa} = \epsilon_j^{(p)} + O(\kappa^2)$);
- There is $\Sigma > \inf \sigma(H)$ (the ionization threshold, $\Sigma + \Sigma^{(p)} + O(\kappa^2)$) s.t. for energies $< \Sigma$ the particles are exponentially localized around the common center of mass.

For energies $> \Sigma$ the system either sheds off locally the excess of energy and descends into a localized state or breaks apart with some of the particles flying off to infinity.



Remark The relation $\epsilon_0 < \epsilon_0^{(p)}$ is due to the fact that the electron surrounded by clouds of photons become heavier.

3.4 Approach

The main steps in our analysis of the spectral structure of the quantum Hamiltonian H are:

- Perform a new canonical transformation (a generalized Pauli-Fierz transform, see Sect. 2.2 above)

$$H \to \tilde{H} := e^{-i\Phi(q_x)} H e^{i\Phi(q_x)},$$

in order to bring H to a more convenient form for our analysis;

- Apply the spectral renormalization group (RG) on new – momentum anisotropic – Banach spaces.

The main ideas of the spectral RG are as follows:

- Pass from a single operator $\tilde{H}_\theta$ to a Banach space $\mathcal{B}$ of Hamiltonian-type operators;
- Construct a map, $\mathcal{R}_\rho$, (RG transformation) on $\mathcal{B}$, with the following properties:

(a) $\mathcal{R}_\rho$ is 'isospectral';
(b) $\mathcal{R}_\rho$ removes the photon degrees of freedom related to energies $\geq \rho$.

- Relate the dynamics of semi-flow, $\mathcal{R}_\rho^n, n \geq 1$, (called renormalization group) to spectral properties of individual operators in $\mathcal{B}$.

4 Minimal Velocity

Results We define the photon velocity in terms of its space-time (and sometimes phase-space-time) localization. In a quantum theory this is formulated in terms of quantum localization observables and related to quantum probabilities. We describe the photon position by the operator $y := i\nabla_k$ on $L^2(\mathbb{R}^3)$, canonically conjugate to the photon momentum k. To test the photon localization, we use the observables $\mathrm{d}\Gamma(\mathbf{1}_S(y))$, where $\mathbf{1}_S(y)$ denotes the characteristic function of a subset S of $\mathbb{R}^3$ and $\mathrm{d}\Gamma(\tau)$ denotes the lifting of a one-photon operator τ to the photon Fock space, $\mathrm{d}\Gamma(\tau)|_{\mathbb{C}} = 0$ for $n = 0$ and, for $n \geq 1$,

$$\mathrm{d}\Gamma(\tau)_{|\otimes_s^n \mathfrak{h}} = \sum_{j=1}^{n} \underbrace{1 \otimes \cdots \otimes 1}_{j-1} \otimes \tau \otimes \underbrace{1 \otimes \cdots \otimes 1}_{n-j}. \tag{15}$$

(See Supplement I for the expression of $\mathrm{d}\Gamma(\tau)$ in terms of $a_\lambda(k)$ and $a_\lambda^*(k)$. Note that $H_f = \mathrm{d}\Gamma(\omega)$.) We also use the localization observables $\Gamma(\mathbf{1}_S(y))$, where $\Gamma(\chi)$ is the lifting of a one-photon operator χ (e.g. a smoothed out characteristic function of y) to the photon Fock space, defined by

$$\Gamma(\chi) = \oplus_{n=0}^{\infty}(\otimes^n \chi), \tag{16}$$

(so that $\Gamma(e^b) = e^{\mathrm{d}\Gamma(b)}$), and then to the space of the total system. Let also $T_h = \Gamma(\tau_h)$, with $\tau_h : f(y) \to f(h^{-1}y)$, where $h \in$ group of rigid motions of $\mathbb{R}^3$. The observables $\mathrm{d}\Gamma(\mathbf{1}_S(y))$ and $\Gamma(\mathbf{1}_S(y))$ have the following natural properties:

- $\mathrm{d}\Gamma(\mathbf{1}_{S_1 \cup S_2}(y)) = \mathrm{d}\Gamma(\mathbf{1}_{S_1}(y)) + \mathrm{d}\Gamma(\mathbf{1}_{S_2}(y))$ and $\Gamma(\mathbf{1}_{S_1}(y))\Gamma(\mathbf{1}_{S_2}(y)) = P_\Omega$, for S_1 and S_2 disjoint, where P_Ω denotes the projection onto the vacuum sector,
- $T_u X_S(y) T_u^{-1} = X_{u^{-1}S}(y)$, where $X_S(y)$ stands for either $\mathrm{d}\Gamma(\mathbf{1}_S(y))$ or $\Gamma(\mathbf{1}_S(y))$.

The observables $\mathrm{d}\Gamma(\mathbf{1}_S(y))$ can be interpreted as giving the number of photons in Borel sets $S \subset \mathbb{R}^3$. They are closely related to those used in [41, 48, 63] (and discussed earlier in [65] and [1]) and are consistent with a theoretical description of the detection of photons (usually via the photoelectric effect, see e.g. [66]). The quantity $\langle \psi, \Gamma(\mathbf{1}_S(y))\psi\rangle$ is interpreted as the probability that the photons are in the set S in the state ψ. This said, we should mention that the subject of photon localization is still far from being settled. (The issue of localizability of photons is a tricky one and has been intensely discussed in the literature since the 1930 and 1932 papers by Landau and Peierls [62] and Pauli [68] (see also a review in [60]). A set of axioms for localization observables was proposed by Newton and Wigner [67] and Wightman [80] and further generalized by Jauch and Piron [59]. Observables describing localization of massless particles, satisfying the Jauch-Piron version of the Wightman axioms, were constructed by Amrein in [1].)

The fact that for photons the observables we use depend on the choice of polarization vector fields, $\varepsilon_\lambda(k)$, $\lambda = 1, 2$, which are not smooth, is not an impediment here as our results imply analogous results for e.g. localization observables of Mandel [65] and of Amrein and Jauch and Piron [1, 59]: $\mathrm{d}\Gamma(f_S^{\mathrm{man}})$ and $\mathrm{d}\Gamma(f_S^{\mathrm{ajp}})$, where $f_S^{\mathrm{man}} := P^\perp \mathbf{1}_S(y) P^\perp$ and $f_S^{\mathrm{ajp}} := \mathbf{1}_S(y) \cap P^\perp$, respectively, acting in the Fock space based on the space $\mathfrak{h} = \mathrm{L}^2_{\mathrm{transv}}(\mathbb{R}^3; \mathbb{C}^3) := \{f \in \mathrm{L}^2(\mathbb{R}^3; \mathbb{C}^3) : k \cdot f(k) = 0\}$ instead of $\mathfrak{h} = \mathrm{L}^2(\mathbb{R}^3; \mathbb{C}^2)$. Here $P^\perp : f(k) \to f(k) - |k|^{-2} k\, k \cdot f(k)$ is the orthogonal projection on the transverse vector fields and, for two orthogonal projections P_1 and P_2, the symbol $P_1 \cap P_2$ stand for the orthogonal projection on the largest subspace contained in $\mathrm{Ran} P_1$ and $\mathrm{Ran} P_2$. (The polarization vector fields $\varepsilon_\lambda(k)$ can be avoided by using the approach of [64].)

In what follows, $\chi_{\cdot \le 1}$ denotes a smoothed out characteristic function of the interval $(-\infty, 1]$, that is it is in $\mathrm{C}^\infty(\mathbb{R})$, non-increasing, equal to 1 if $x \le 1/2$ and equal to 0 if $x \ge 1$. Moreover, $\chi_{\cdot \ge 1} := \mathbf{1} - \chi_{\cdot \le 1}$ and $\chi_{\cdot = 1}$ stands for the derivative of $\chi_{\cdot \ge 1}$. Given a self-adjoint operator a and a real number α, we write $\chi_{a \le \alpha} := \chi_{\frac{a}{\alpha} \le 1}$, and likewise for $\chi_{a \ge \alpha}$ and $\chi_{a = \alpha}$. We say that the system obeys the *minimal photon velocity bound* if the Schrödinger evolution, $\psi_t = e^{-itH}\psi_0$, obeys the estimates

$$\int_1^\infty dt\, t^{-\alpha'} \left\| \mathrm{d}\Gamma(\chi_{\frac{|y|}{ct^\alpha} = 1})^{\frac{1}{2}} \psi_t \right\|^2 \lesssim \|\psi_0\|_0^2, \tag{17}$$

for some norm $\|\psi_0\|_0$, some $0 < \alpha' \le 1$, and for any $\alpha > 0$ and $c > 0$ such that either $\alpha < 1$, or $\alpha = 1$ and $c < 1$. In other words there are no photons which either diffuse or propagate with speed < 1. The *maximal velocity estimate*, as proven in [11], states that, for any $c' > 1$,

$$\left\| \mathrm{d}\Gamma\big(\chi_{\frac{|y|}{c't} \ge 1}\big)^{\frac{1}{2}} \psi_t \right\| \lesssim t^{-\gamma} \left\| (\mathrm{d}\Gamma(\langle y \rangle) + 1)^{\frac{1}{2}} \psi_0 \right\|, \tag{18}$$

with $\gamma < \min(\frac{1}{2}(1 - \frac{1}{c'}), \frac{1}{10})$ for (3), and $\gamma < \min(\frac{\mu}{2}(\frac{c'-1}{2c'-1}), \frac{1}{2+\mu})$ for (48)–(50) with $\mu > 0$.

As we discussed above, the operator H has *a unique ground state* (denoted here as $\Phi_{\rm gs}$) and that generically (e.g. under the Fermi Golden Rule condition), H has no eigenvalues in the interval $(E_{\rm gs}, a]$, where $a < \Sigma$ can be taken arbitrarily close to Σ, depending on the coupling constant and on whether the particle system has an infinite number of eigenvalues accumulating to its ionization threshold (see [9, 44, 47]). *We assume* that this is exactly the case:

Fermi's Golden Rule ([7, 8]) holds for all excited eigenvalues $\leq a$ of H_p. (19)

Assumption (19) means that for every excited eigenvalue $e_j \leq a$ of H_p, we have

$$\Pi_j W \mathrm{Im}((H_0 - e_j - i0^+)^{-1}\bar{\Pi}_j) W \Pi_j \geq c_j \Pi_j, \quad c_j > 0, \tag{20}$$

where $H_0 := H_p + H_f$ (for either model), $W := H - H_0$, Π_j denotes the projection onto the eigenspace of H_0 associated to e_j and $\bar{\Pi}_j := \mathbf{1} - \Pi_j$. In fact, there is an explicit representation of (20). Since it differs slightly for different models, we present it for the phonon one, assuming for simplicity that the eigenvalue e_j is simple:

$$\int \langle \phi_j, g^*(k) \mathrm{Im}(H_p + \omega(k) - e_j - i0^+)^{-1} g(k) \phi_j \rangle dk > 0, \tag{21}$$

where ϕ_j is an eigenfunction of H_p corresponding to the eigenvalue e_j and the inner product is in the space $\mathcal{H}_p$. It is clear from (21) that Fermi's Golden Rule holds generally, with a very few exceptions.

Let $N := \mathrm{d}\Gamma(\mathbf{1})$ be the photon (or phonon) number operator and $N_\rho := \mathrm{d}\Gamma(\omega^{-\rho})$ be the photon (or phonon) low momentum number operator. In what follows we let ψ_t denote the Schrödinger evolution, $\psi_t = e^{-itH}\psi_0$, i.e. the solution of the Schrödinger equation (1), with an initial condition ψ_0, satisfying $\psi_0 = f(H)\psi_0$, with $f \in \mathrm{C}_0^\infty((-\infty, \Sigma))$. More precisely, we will consider the following sets of initial conditions

$$\Upsilon_\rho := \left\{ \psi_0 \in f(H) D(N_\rho)^{\frac{1}{2}}, \text{ for some } f \in \mathrm{C}_0^\infty((-\infty, \Sigma)) \right\},$$

and

$$\Upsilon_\# := \left\{ \psi_0 \in f(H) \big(D(\mathrm{d}\Gamma(\langle y \rangle)) \cap D(\mathrm{d}\Gamma(b)^2) \big), \text{ for some } f \in \mathrm{C}_0^\infty((E_{\rm gs}, a]) \right\},$$

where $b := \frac{1}{2}(k \cdot y + y \cdot k)$ and $a < \Sigma$ is given by Assumption (19).

For $A \geq -C$, we denote $\|\psi_0\|_A := \|(A + C + 1)^{\frac{1}{2}}\psi_0\|$. We define $\nu_\rho \geq 0$ as the smallest real number satisfying the inequality

$$\langle \psi_t, N_\rho \psi_t \rangle \lesssim t^{\nu_\rho} \|\psi_0\|_\rho^2, \tag{22}$$

for any $\psi_0 \in \mathrm{Ran}\, E_{(-\infty,\Sigma)}(H)$, where $\|\psi\|_\rho^2 := \|\psi\|_{N_\rho}^2$. It was shown in [11] that, for any $-1 \le \rho \le 1$, the inequality (22) is satisfied with

$$\nu_\rho \le \frac{1+\rho}{2+\mu}. \tag{23}$$

(This generalizes an earlier result due to [48].) Also, the bound $\|\psi_t\|_{H_f} \lesssim \|\psi_0\|_H$ shows that (22) holds for $\rho = -1$ with $\nu_{-1} = 0$. With ν_ρ defined by (22), we prove the following two results.

Theorem 4.1 (Minimal photon velocity bound) *Consider the Hamiltonian* (3). *Let either* $\alpha = 1$ *and* $c < 1$ *or*

$$\max\left(\frac{1}{6}(5+\nu_1-\nu_0), \frac{3}{4}\right) < \alpha < 1. \tag{24}$$

Then for any initial condition $\psi_0 \in \Upsilon_1$, *the Schrödinger evolution,* ψ_t, *satisfies, for any* $a > 1$, *the following estimate*

$$\int_1^\infty dt\, t^{-\alpha-a\nu_0} \|\mathrm{d}\Gamma(\chi_{\frac{|y|}{ct^\alpha}=1})^{\frac{1}{2}}\psi_t\|^2 \lesssim \|\psi_0\|_1^2. \tag{25}$$

For the coupling function g, we introduce the norm

$$\langle g\rangle := \sum_{|\alpha|\le 2} \|\eta_1 \eta_2^{|\alpha|}\partial^\alpha g\|_{L^2(\mathbb{R}^3,\mathcal{H}_p)}.$$

We have

Theorem 4.2 (Weak minimal photon escape velocity estimate) *Consider the Hamiltonian* (3) *with the coupling constants* κ_j *sufficiently small. Assume* (19), $\nu_0 + \nu_1 < \alpha < 1 - \nu_0$ *and* $c > 0$. *Then for any initial condition* $\psi_0 \in \Upsilon_\#$, *the Schrödinger evolution,* ψ_t, *satisfies the estimate*

$$\left\|\Gamma(\chi_{\frac{|y|}{ct^\alpha}\le 1})\psi_t\right\| \lesssim t^{-\gamma}\left(\|\psi_0\|_{\mathrm{d}\Gamma(\langle y\rangle)} + \|\psi_0\|_{\mathrm{d}\Gamma(b)^2}\right), \tag{26}$$

where $\gamma < \frac{1}{2}\min(1-\alpha-\nu_0, \frac{1}{2}(\alpha-\nu_0-\nu_1))$.

Remarks

(1) The estimate (25) is sharp if $\nu_0 = 0$. Assuming this and taking $\nu_1 \le 1/2$, the conditions on α in Theorems 4.1 and 4.2 become $\alpha > 11/12$, and $1/2 < \alpha < 1$, respectively.

(2) The estimate (26) states that, as $t \to \infty$, with probability $\to 1$, either all photons are attached to the particle system in the combined ground state, or at least one photon departs the particle system with the distance growing at least as $\mathcal{O}(t^\alpha)$.

(Remember that the set $\Upsilon_\#$ excludes the ground state, and the exited states below Σ are excluded by the condition (19).)

(3) With some more work, one can remove the assumption (19) and relax the condition on ψ_0 in Theorem 4.2 to the natural one: $\psi_0 \in P_\Sigma D(\mathrm{d}\Gamma(\langle y\rangle))$, where P_Σ is the spectral projection onto the orthogonal complement of the eigenfunctions of H with corresponding eigenvalues in the interval $(-\infty, \Sigma)$.

(4) For the spin-boson model, a uniform bound, $\langle \psi_t, e^{\delta N}\psi_t\rangle \leq C(\psi_0) < \infty$, $\delta > 0$, on the number of photons, on a dense set of ψ_0's, without controlling the dependence of the constant $C(\psi_0)$ on this dense set, was recently proven in [20]. See [35] for a discussion of such bounds.

Approach One uses the method of propagation observables, originating in the many body scattering theory ([23, 49, 58, 75, 76, 81], see [25, 57] for a textbook exposition and a more recent review) and extended to the non-relativistic quantum electrodynamics in [26, 40–43, 48] and to the $P(\varphi)_2$ quantum field theory, in [27]. It was used in [11] to prove the *maximal velocity estimate*, which states that, for any $c' > 1$,

$$\left\|\mathrm{d}\Gamma\big(\chi_{\frac{|y|}{c't}\geq 1}\big)^{\frac{1}{2}}\psi_t\right\| \lesssim t^{-\gamma}\left\|(\mathrm{d}\Gamma(\langle y\rangle)+1)^{\frac{1}{2}}\psi_0\right\|, \tag{27}$$

with $\gamma < \min(\frac{1}{2}(1-\frac{1}{c'}), \frac{1}{10})$. We present an abstract description of the method of propagation observables in Appendix Appendix 4:.

First, we prove a version of the minimal photon escape velocity estimates formulated in terms of the self-adjoint operators b_ϵ defined as

$$b_\epsilon := \frac{1}{2}(v(k)\cdot y + y\cdot v(k)),$$

where $v(k) := \frac{k}{\omega+\epsilon}$, for $\epsilon = t^{-\kappa}$, with some $\kappa > 0$. Since the vector field $v(k)$ is Lipschitz continuous and therefore generates a global flow, the operator b_ϵ is self-adjoint. Namely, we show the minimal photon escape velocity estimate of the form

$$\int_1^\infty dt\, t^{-\alpha'}\left\|\mathrm{d}\Gamma(\chi_{\frac{b_\epsilon}{ct^\alpha}=1})^{\frac{1}{2}}\psi_t\right\|^2 \lesssim \|(N_1+1)^{\frac{1}{2}}\psi_0\|^2, \tag{28}$$

for some α' and α satisfying $0 < \alpha \leq \alpha' \leq 1$, and

$$\left\|\Gamma(\chi_{\frac{b_\epsilon}{ct^\alpha}\leq 1})^{\frac{1}{2}}\psi_t\right\|^2 \lesssim t^{-\delta}\big(\|(\mathrm{d}\Gamma(\langle y\rangle)+1)^{\frac{1}{2}}\psi_0\|^2 + \|(\mathrm{d}\Gamma(b)+1)\psi_0\|^2\big), \tag{29}$$

for some $\alpha \leq 1$ and $\delta > 0$, where $b = \frac{1}{2}(k\cdot y + y\cdot k)$ and $\Gamma(\chi)$ is the lifting of a one-photon operator χ defined in (16). Then we pass from the operators b_ϵ to $|y|$.

Using b_ϵ, rather than the operator $b_0 := \frac{1}{2}(\frac{k}{\omega}\cdot y + y\cdot\frac{k}{\omega})$ used in [48], avoids some technicalities.

Remark At the expense of slightly lengthier computations, but gaining simpler technicalities, one can also modify b_ϵ to make it bounded, by multiplying it with the cut-off function $\chi_{\frac{|y|}{c'_I}\leq 1}$ with $c' > 1$, such that the maximal velocity estimate (27) holds, or use the smooth vector field $v(k) = \frac{k}{\sqrt{\omega^2+\epsilon^2}}$, instead of $v(k) = \frac{k}{\omega+\epsilon}$.

5 Scattering

Results We begin with giving the precise definition of asymptotic completeness. We define the space $\mathcal{H}_{\rm fin} := \mathcal{H}_p \otimes \mathcal{F}_{\rm fin} \otimes \mathcal{F}_{\rm fin}$, where $\mathcal{F}_{\rm fin} \equiv \mathcal{F}_{\rm fin}(\mathfrak{h})$ is the subspace of $\mathcal{F}$ consisting of vectors $\Psi = (\psi_n)_{n=0}^\infty \in \mathcal{F}$ such that $\psi_n = 0$, for all but finitely many n, and the (*scattering*) map $I : \mathcal{H}_{\rm fin} \to \mathcal{H}$ as the extension by linearity of the map (see [26, 41, 56])

$$I : \Phi \otimes \prod_1^n a^*(h_i)\Omega \to \prod_1^n a^*(h_i)\Phi, \tag{30}$$

for any $\Phi \in \mathcal{H}_p \otimes \mathcal{F}_{\rm fin}$ and for any $h_1, \dots h_n \in \mathfrak{h}$. Here $a^\#(h)$ are the creation and annihilation operators evaluated on a function h, see Supplement II. Another useful representation of I is

$$I : \Phi \otimes f \to \binom{p+q}{p}^{1/2} \Phi \otimes_s f, \tag{31}$$

for any $\Phi \in \mathcal{H}_p \otimes (\otimes_s^p \mathfrak{h})$ and $f \in \otimes_s^q \mathfrak{h}$. (We call I the *Hübner-Spohn scattering map*.) As already clear from (30), the operator I is unbounded.

Now, it is known (see [8, 51]) that the operator H has *a unique ground state* (denoted here as $\Phi_{\rm gs}$). Let $E_{\rm gs}$ be the ground state energy and $E_{\rm gs} < a < \Sigma$ be such that the Hamiltonian H has no eigenvalues in the interval $(E_{\rm gs}, a]$. We say that asymptotic completeness holds on the interval $\Delta = [E_{\rm gs}, a]$, if, for every $\epsilon > 0$ and $\phi_0 \in {\rm Ran}\chi_\Delta(H)$, there is $\phi_{0\epsilon} \in \mathcal{F}_{\rm fin}$ s.t.

$$\limsup_{t\to\infty} \|e^{-iHt}\phi_0 - I(e^{-iE_{\rm gs}t}P_{\rm gs} \otimes e^{-iH_f t}\chi_{\Delta'}(H_f))\phi_{0\epsilon}\| = \mathcal{O}(\epsilon), \tag{32}$$

where $\Delta' = [0, a - E_{\rm gs}]$ and $P_{\rm gs}$ is the orthogonal projection onto $\Phi_{\rm gs}$.

Generically (e.g. under the Fermi Golden Rule condition, (19)), H has no eigenvalues in the interval $(E_{\rm gs}, a]$, where $a < \Sigma$ can be taken arbitrarily close to Σ, depending on the coupling constant and on whether the particle system has an infinite number of eigenvalues accumulating to its ionization threshold (see [9, 44, 47]). *We assume* that this is exactly the case. Assumption (19) was stated rigorously in (20) and discussed after that formula. As was mentioned above, Fermi's Golden Rule holds generally, with a very few exceptions. Treatment of

the (exceptional) situation when excited embedded eigenvalues do occur requires, within our approach, proving a delicate estimate $\|P_\Omega f(H)\| \lesssim \langle g \rangle$, where P_Ω denotes the projection onto $\mathcal{H}_p \otimes \Omega$ (where $\Omega := 1 \oplus 0 \oplus \dots$ is the vacuum in $\mathcal{F}$) and $f \in \mathrm{C}_0^\infty((E_{\mathrm{gs}}, \Sigma) \setminus \sigma_{\mathrm{pp}}(H))$, uniformly in $\mathrm{dist}\,(\mathrm{supp} f, \sigma_{\mathrm{pp}}(H))$.

Let $N := \mathrm{d}\Gamma(\mathbf{1})$ be the photon (or phonon) number operator and $N_\rho := \mathrm{d}\Gamma(\omega^{-\rho})$ be the photon (or phonon) low momentum number operator. In what follows we let ψ_t denote the Schrödinger evolution, $\psi_t = e^{-itH}\psi_0$, i.e. the solution of the Schrödinger equation (1), with an initial condition ψ_0, satisfying $\psi_0 = f(H)\psi_0$, with $f \in \mathrm{C}_0^\infty((-\infty, \Sigma))$. We have

Theorem 5.1 (Asymptotic Completeness) *Consider the Hamiltonian* (3) *with the coupling constants κ_j sufficiently small. Assume* (19) *and suppose that either*

$$\|N^{\frac{1}{2}}\psi_t\| \lesssim \|N^{\frac{1}{2}}\psi_0\| + \|\psi_0\|, \tag{33}$$

for any $\psi_0 \in f(H)D(N^{1/2})$, with $f \in \mathrm{C}_0^\infty((E_{\mathrm{gs}}, \Sigma))$, uniformly in $t \in [0, \infty)$, or

$$\|N_1^{\frac{1}{2}}\psi_t\| \lesssim 1, \tag{34}$$

uniformly in $t \in [0, \infty)$, for any $\psi_0 \in \mathcal{D}$, where $\mathcal{D}$ is such that

$$\mathcal{D} \cap D(\mathrm{d}\Gamma(\omega^{-1/2}\langle y \rangle \omega^{-1/2})^{\frac{1}{2}})$$

is dense in $\mathrm{Ran}\, E_{(-\infty,\Sigma)}(H)$. *Then asymptotic completeness holds on* $[E_{\mathrm{gs}}, a]$.

Assumption (33) can be replaced by the slightly weaker hypothesis that there exist $1/2 \leq \delta_1 \leq \delta_2$ such that for any $\psi_0 \in f(H)D(N^{\delta_2})$, with $f \in \mathrm{C}_0^\infty((E_{\mathrm{gs}}, \Sigma))$, $\|N^{\delta_1}\psi_t\| \lesssim \|N^{\delta_2}\psi_0\| + \|\psi_0\|$, uniformly in $t \in [0, \infty)$.

The advantage of Assumption (34) is that the uniform bound on

$$N_1 = \mathrm{d}\Gamma(\omega^{-1})$$

is required to hold only for an *arbitrary* dense set of initial states and, as a result, can be verified for the massless spin-boson model by modifying slightly the proof of [20] (see the discussion below). Hence asymptotic completeness in this case holds with no implicit conditions.

As we see from the results above, the uniform bounds, (33) or (34), on the number of photons (or phonons) emerge as the remaining stumbling blocks to proving asymptotic completeness without qualifications. The difficulty in proving these bounds for massless fields is due to the same infrared problem which pervades this field and which was successfully tackled in other central issues, such as the theory of ground states and resonances (see [4, 73] for reviews), the local decay and the maximal velocity bound.

For massive bosons (e.g. optical phonons), the inequality (33) (as well as (22), with $\nu_0 = 0$) is easily proven and the proof below simplifies considerably as well.

In this case, the result is unconditional. It was first proven in [26] for models with confined particles, and in [41] for Rayleigh scattering.

As was mentioned above, for the spin-boson model, a uniform bound

$$\langle \psi_t, e^{\delta N} \psi_t \rangle \leq C(\psi_0) < \infty, \ \delta > 0$$

on the number of photons, on a dense set of ψ_0's, was recently proven in the remarkable paper [20].

To verify (34) for the spin-boson model, with $\mu > 0$, we proceed precisely in the same way as in [20], but using a stronger condition on the decay of correlation functions,

$$\int_0^\infty dt\,(1+t)^\alpha |h(t)| < \infty, \quad \text{with} \quad h(t) := \int_{\mathbb{R}^3} dk\, e^{-it|k|}(1+|k|^{-1})|g(k)|^2, \tag{35}$$

for some $\alpha \geq 1$, instead of Assumption A of [20], and bounding the observable $(1+\kappa N_{1/2})^2$ instead of $e^{\kappa N}$. Assumption C of [20] on initial states has to be replaced in the same manner. Assuming that our condition (34) on the coupling function g is satisfied with $\mu > 0$ (and $\eta = 1$), we see that (35) holds with $\alpha = 1 + 2\mu$.

The form of the observable $e^{\kappa N}$ enters [20] through the estimate $\|K_{u,v}\|_\diamond \leq C|h(u-v)|$ of the operator $K_{u,v}$ defined in [20, (3.4)] and the standard estimate [20, (4.36)]. Both extend readily to our case (the former with $h(t)$ given in (35)). Moreover, [20, (4.36)] is used in the proof that pressure vanishes – Eq. (4.39) in [20] – and the latter also follows from Proposition A.1 of [35]. (One can also use the observable $e^{-\mathrm{d}\Gamma(\lambda \ln \omega)}$ – equal to $\Gamma(\omega^{-\lambda})$, see (16) below for the definition of $\Gamma(\chi)$ – and analyticity, rather than perturbation, in λ.)

Approach Once the minimal velocity estimates are proven, the first step in the proof of asymptotic completeness is to decouple the photons in the expanding ball $\{b_\epsilon \leq ct^\alpha\}$ from those inside $\{b_\epsilon \geq ct^\alpha\}$. To this end we use the second quantization, $\Gamma(j) : \Gamma(\mathfrak{h}) \to \alpha(\mathfrak{h} \oplus \mathfrak{h})$ of a partition of unity $j : h \to j_0 h \oplus j_\infty h$ on the one-photon space, $j : \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$, with j_0 localizing a photon to a region $\{b_\epsilon \leq ct^\alpha\}$, and j_∞, to $\{b_\epsilon \geq ct^\alpha\}$, and satisfying $j_0^2 + j_\infty^2 = \mathbf{1}$. Defining the adjoint map $j^* : h_0 \oplus h_\infty \to j_0^* h_0 + j_\infty^* h_\infty$, so that $j^* j = j_0^2 + j_\infty^2 = \mathbf{1}$, and using $\Gamma(j)^* \Gamma(j) = \Gamma(j^* j)$, we see that $\Gamma(j)^* \Gamma(j) = \mathbf{1}$.

The partition $\Gamma(j)$ is further refined as ([26, 41]) $\check{\Gamma}(j) := U\Gamma(j) : \Gamma(\mathfrak{h}) \to \Gamma(\mathfrak{h}) \otimes \Gamma(\mathfrak{h})$, where $U : \Gamma(\mathfrak{h} \oplus \mathfrak{h}) \to \Gamma(\mathfrak{h}) \otimes \Gamma(\mathfrak{h})$ is the unitary map defined through the relations $U\Omega = \Omega \otimes \Omega$, $Ua^*(h) = [a^*(h_1) \otimes \mathbf{1} + \mathbf{1} \otimes a^*(h_2)]U$, for any $h = (h_1, h_2) \in \mathfrak{h} \oplus \mathfrak{h}$, and is then lifted from the Fock space $\mathcal{F} = \Gamma(\mathfrak{h})$ to the full state space $\mathcal{H} = \mathcal{H}_p \otimes \mathcal{F}$. As above, $\check{\Gamma}(j)^* \check{\Gamma}(j) = \mathbf{1}$. (We call $\check{\Gamma}(j)$ the *Dereziński-Gérard partition of unity* .) Using $\check{\Gamma}(j)$, we define the Deift-Simon wave operators ([22, 26, 41, 74]),

$$W_\pm := \operatorname*{s-lim}_{t \to \pm\infty} e^{i\hat{H}t} \check{\Gamma}(j) e^{-iHt}, \tag{36}$$

where $\hat{H} := H \otimes \mathbf{1} + \mathbf{1} \otimes H_f$, on the auxiliary space $\hat{\mathcal{H}} := \mathcal{H} \otimes \mathcal{F}$. Next, the existence and the properties of the Deift-Simon wave operators (36) on $\mathrm{Ran}_{(-\infty,\Sigma)}(H)$ is equivalent to the existence and the properties of the modified Deift-Simon wave operators

$$W_{\pm}^{(mod)} := \underset{t \to \pm\infty}{\text{s-lim}} \left(e^{-i\Phi(q_x)} \otimes \mathbf{1}\right) e^{it\hat{H}} \check{\Gamma}(j) e^{-itH} e^{i\Phi(q_x)}, \tag{37}$$

on $\mathrm{Ran}_{(-\infty,\Sigma)}(\tilde{H})$. Here, recall, $\tilde{H} = e^{-i\Phi(q_x)} H e^{i\Phi(q_x)}$ is defined in (7)–(8) and given explicitly in (9).

To prove the existence of $W_{\pm}^{(mod)}$, we use the relation

$$\check{\Gamma}(j) a^{\#}(h) = \hat{a}^{\#}(h) \check{\Gamma}(j),$$

where $\hat{a}^{\#}(h) := a^{\#}(j_0 h) \otimes \mathbf{1} + \mathbf{1} \otimes a^{\#}(j_\infty h)$, with $a^{\#}$ standing for a or a^*, which gives $\check{\Gamma}(j)\Phi(h) = \hat{\Phi}(h)\check{\Gamma}(j)$, where

$$\hat{\Phi}(h) := \Phi(j_0 h) \otimes \mathbf{1} + \mathbf{1} \otimes \Phi(j_\infty h), \tag{38}$$

which in turn implies that

$$\check{\Gamma}(j) e^{i\Phi(h)} = e^{i\hat{\Phi}(h)} \check{\Gamma}(j). \tag{39}$$

Therefore

$$\begin{aligned} \left(e^{-i\Phi(q_x)} \otimes \mathbf{1}\right) e^{it\hat{H}} \check{\Gamma}(j) e^{-itH} e^{i\Phi(q_x)} &= \left(e^{-i\Phi(q_x)} \otimes \mathbf{1}\right) e^{it\hat{H}} e^{i\hat{\Phi}(q_x)} \check{\Gamma}(j) e^{-it\tilde{H}} \\ &= e^{it\hat{H}^{(\mathrm{mod})}} \check{\Gamma}(j) e^{-it\tilde{H}} + \mathrm{Rem}_t, \end{aligned} \tag{40}$$

where $\hat{H}^{(\mathrm{mod})} := \tilde{H} \otimes \mathbf{1} + \mathbf{1} \otimes H_f$ and

$$\mathrm{Rem}_t := \left(e^{-i\Phi(q_x)} \otimes \mathbf{1}\right) e^{it\hat{H}} \left(e^{i\hat{\Phi}(q_x)} - e^{i\Phi(q_x)} \otimes \mathbf{1}\right) \check{\Gamma}(j) e^{-it\tilde{H}}.$$

It is a matter of technical estimates (see [35]) to show that

$$\underset{t \to \pm\infty}{\text{s-lim}}\, \mathrm{Rem}_t = 0. \tag{41}$$

The equations (36), (40) and (41) imply

$$W_{\pm}^{(mod)} = \underset{t \to \pm\infty}{\text{s-lim}}\, e^{it\hat{H}^{(\mathrm{mod})}} \check{\Gamma}(j) e^{-it\tilde{H}}. \tag{42}$$

Now, to prove the existence of the limits in (42), we use the standard Cook argument by introducing $W(t) := e^{it\hat{H}^{(\mathrm{mod})}}\check{\Gamma}(j)e^{-it\tilde{H}}$ and writing

$$W(t') - W(t) = \int_t^{t'} ds\, \partial_s W(s). \tag{43}$$

It is easy to compute the derivative on the r.h.s. $\partial_t W(t) = e^{i\hat{H}t}Ge^{-iHt}$, where $G := i(\hat{H}\check{\Gamma}(j) - \check{\Gamma}(j)H) + \partial_t\check{\Gamma}(j)$, and, after some lengthy manipulations (see [35]) to reduce the problem to the estimate of the same integral as the one appearing in the first minimal velocity estimate for b_ϵ. Then the latter estimate implies that the limits in (42) exist.

The existence of the Deift-Simon wave operators implies that

$$\psi_t = \check{\Gamma}(j)^* e^{-i\hat{H}t}e^{i\hat{H}t}\check{\Gamma}(j)e^{-iHt}\psi_0 = \check{\Gamma}(j)^* e^{-i\hat{H}t}\phi_0 + o_t(1), \tag{44}$$

where $\phi_0 := W_+\psi_0$. Since $e^{-i\hat{H}t} = e^{-iHt} \otimes e^{-iH_f t}$, we see that the first term on the r.h.s. describes the photons in the expanding ball $\{b_\epsilon \leq ct^\alpha\}$ decoupled from those inside $\{b_\epsilon \geq ct^\alpha\}$.

Next, let $\Delta = [E_{\mathrm{gs}}, a] \subset \mathbb{R}$, where $a < \Sigma$, and $\Delta' = [0, a - E_{\mathrm{gs}}]$. The existence of W_+ implies the property $W_+\chi_\Delta(H) = \chi_\Delta(\hat{H})W_+$, which gives $\phi_0 = \chi_\Delta(\hat{H})\phi_0$ if $\psi_0 \in \mathrm{Ran}(\chi_\Delta(H))$. The latter relation together with

$$\chi_\Delta(\hat{H}) = (\chi_\Delta(H) \otimes \chi_{\Delta'}(H_f))\chi_\Delta(\hat{H})$$

implies $\phi_0 = \big(\chi_\Delta(H) \otimes \chi_{\Delta'}(H_f)\big)\phi_0$. Next, we use that for all $\epsilon > 0$, there is $\delta = \delta(\epsilon) > 0$, such that

$$\big\|(\chi_\Delta(H) \otimes \mathbf{1})\phi_0 - (\chi_{\Delta_\epsilon}(H) \otimes \mathbf{1})\phi_0 - (P_{\mathrm{gs}} \otimes \mathbf{1})\phi_0\big\| \leq \epsilon, \tag{45}$$

where $\Delta_\epsilon = [E_{\mathrm{gs}} + \delta, a]$ and P_{gs} is the orthogonal projection onto the ground state of H. Applying this equation and the relations $e^{-i\hat{H}t} = e^{-iHt} \otimes e^{-iH_f t}$ and $e^{-iHt}P_{\mathrm{gs}} = e^{-iE_{\mathrm{gs}}t}P_{\mathrm{gs}}$ to (44) gives, after some manipulations with energy cut-offs,

$$\psi_t = \check{\Gamma}(j)^*\big(e^{-iE_{\mathrm{gs}}t}P_{\mathrm{gs}} \otimes e^{-iH_f t}\chi_{\Delta'}(H_f)\big)\phi_0 + \check{\Gamma}(j)^*\phi_t + \mathcal{O}(\epsilon) + o_t(1), \tag{46}$$

where $\phi_t = \big(e^{-iHt}\chi_{\Delta_\epsilon}(H) \otimes e^{-iH_f t}\chi_{\Delta'}(H_f)\big)\phi_0$ and $\mathcal{O}(\epsilon)$ and $C(\epsilon)o_t(1)$ denote L^2-functions bounded by $C\epsilon$ and tending to 0 as $t \to \infty$, respectively.

Now, let $(\tilde{j}_0, \tilde{j}_\infty)$ be localized similarly to (j_0, j_∞) and satisfy

$$j_0\tilde{j}_0 = j_0,\ j_\infty\tilde{j}_\infty = j_\infty.$$

Then, as shown below, the adjoint $\check{\Gamma}(j)^*$ to the operator $\check{\Gamma}(j)$ can be represented as $\check{\Gamma}(j)^* = \check{\Gamma}(j)^*\big(\Gamma(\tilde{j}_0) \otimes \Gamma(\tilde{j}_\infty)\big)$. Using this equation in (44) and using that $\big(\Gamma(\tilde{j}_0) \otimes$

1) $\phi_t \to 0$, as $t \to \infty$, by the second minimal velocity estimate for b_ϵ, we see that the second term on the r.h.s. of (46) vanishes, as $t \to \infty$.

To conclude the sketch of the proof of asymptotic completeness, we pass from the operator $\check{\Gamma}(j)^*$ to the (*scattering*) map I defined in (30)–(31). To this end we use the formula $\check{\Gamma}(j)^* = I\Gamma(j_0^*) \otimes \Gamma(j_\infty^*)$, for any operator $j : h \to j_0 h \oplus j_\infty h$, and some elementary estimates in order to remove $\Gamma(j_0^*) \otimes \Gamma(j_\infty^*)$.

6 Conclusion

Apart from the vacuum polarization, the non-relativistic QED provides a good qualitative description of the physical phenomena related to the interaction of quantized electrons and nuclei and the electro-magnetic field.

The quantitative results though are still missing. Does the free parameter, m (or κ), suffice to give a good fit with the experimental data, say, on the radiative corrections? Another important open question is the behaviour of the theory in the ultra-violet cut-off.

7 Comments on Literature

The local decay property was proven in [8–10, 13, 44–47], by the combination of the renormalization group and positive commutator methods. The maximal and minimal velocity estimates were proven in [11] and [36], respectively. For models involving massive bosons fields, some minimal velocity estimates are proven in [26].

In [20], the authors proved relaxation to the ground state and uniform bounds on the number of emitted massless bosons in the spin-boson model. (Importance of both questions was emphasized earlier by Jürg Fröhlich.)

Asymptotic completeness was proven for (a small perturbation of) a solvable model involving a harmonic oscillator (see [2, 78]), and for models involving massive boson fields ([26, 41–43]). Moreover, [48] obtained some important results for massless bosons (the Nelson model) in confined potentials.

Motivated by the many-body quantum scattering, [26, 41–43, 48] defined the main notions of scattering theory on Fock spaces, such as wave operators, asymptotic completeness and propagation estimates.

In [35], asymptotic completeness was proven for Rayleigh scattering on the states for which the expectation of either the photon/phonon number operator, N, or an operator, N_1, testing the photon/phonon infrared behaviour is uniformly bounded on corresponding dense sets. By extending the result of [20] in a straightforward way, [35] have shown that the second of these conditions is satisfied for the spin-boson model. For comparison of this first result with [48], see [35].

A different proof of asymptotic completeness for the massless spin-boson model was given in [21]

Appendix 1: Hamiltonian of the Standard Model

In this appendix we discuss the origin the quantum Hamiltonian H given in (3). To be specific consider an atom or molecule with n electrons interacting with radiation field. In this case the Hamiltonian of the system in our units is given by

$$H(\alpha) = \sum_{j=1}^{n} \frac{1}{2m}(i\nabla_{x_j} - \sqrt{\alpha}A_{\xi'}(x_j))^2 + \alpha U(x) + H_f, \tag{47}$$

where $\alpha U(x)$ is the total Coulomb potential of the particle system, m is the electron bare mass, $\alpha = \frac{e^2}{4\pi\hbar c} \approx \frac{1}{137}$ (the fine-structure constant) and $A_{\xi'}(y)$ is the original vector potential with the ultraviolet cut-off ξ'. Rescaling $x \to \alpha^{-1}x$ and $k \to \alpha^2 k$, we arrive at the Hamiltonian (3), where $\kappa \equiv \kappa_j := \alpha^{3/2}$ and $A(y) = A_\xi(\alpha y)$, with $\xi(k) := \xi'(\alpha^2 k)$. After that we relax the restriction on $U(x)$ by allowing it to be a standard generalized n-body potential (see Sect. 2). Note that though this is not displayed, $A(x)$ does depend on κ. This however does not effect the analysis of the Hamiltonian H. (If anything, this makes certain parts of it simpler, as derivatives of $A(x)$ bring down κ.)

In order not to deal with the problem of center-of-mass motion which is not essential in the present context, we assume that either some of the particles (nuclei) are infinitely heavy (a molecule in the Born-Oppenheimer approximation), or the system is placed in a binding, external potential field. (In the case of the Born-Oppenheimer molecule, the resulting $V(x)$ also depends on the rescaled coordinates of the nuclei, but this does not effect our analysis except of making the complex deformation of the particle system more complicated (see [57]).) This means that the operator H_p has isolated eigenvalues below its essential spectrum. The general case is considered below.

Appendix 2: Phonon Hamiltonian

The results discussed in this review cover also the standard phonon model of solid state physics (see e.g. [61]). The state space for it is given by $\mathcal{H} := \mathcal{H}_p \otimes \mathcal{F}$, where $\mathcal{H}_p$ is the particle state space and $\mathcal{F} \equiv \Gamma(\mathfrak{h}) = \mathbb{C} \oplus_{n=1}^{\infty} \otimes_s^n \mathfrak{h}$ is the bosonic Fock space based on the one-phonon space $\mathfrak{h} := L^2(\mathbb{R}^3, \mathbb{C})$. Its dynamics is generated by the Hamiltonian

$$H := H_p + H_f + I(g), \tag{48}$$

acting on $\mathcal{H}$, where H_p is a self-adjoint particle system Hamiltonian, acting on $\mathcal{H}_p$, and $H_f = \mathrm{d}\Gamma(\omega)$ is the phonon Hamiltonian acting on $\mathcal{F}$, where $\omega = \omega(k)$ is the phonon dispersion law (k is the phonon wave vector). For *acoustic phonons*, $\omega(k) \asymp |k|$ for small $|k|$ and $c \leq \omega(k) \leq c^{-1}$, for some $c > 0$, away from 0, while for *optical phonons*, $c \leq \omega(k) \leq c^{-1}$, for some $c > 0$, for all k. To fix ideas, we consider below only the most difficult case $\omega(k) = |k|$.

The operator $I(g)$ acts on $\mathcal{H}$ and represents an interaction energy, labeled by a coupling family $g(k)$ of operators acting on the particle space $\mathcal{H}_p$. In the simplest case of linear coupling (the dipole approximation in QED or the phonon models), $I(g)$ is given by

$$I(g) := \int (g^*(k) \otimes a(k) + g(k) \otimes a^*(k))dk, \tag{49}$$

where $a^*(k)$ and $a(k)$ are the phonon creation and annihilation operators acting on $\mathcal{F}$, and $g(k)$ is a family of operators on $\mathcal{H}_p$ (coupling operators), for which we assume the following condition

$$\|\eta_1 \eta_2^{|\alpha|} \partial^\alpha g(k)\|_{\mathcal{H}_p} \lesssim |k|^{\mu-|\alpha|} \langle k \rangle^{-2-\mu}, \quad |\alpha| \leq 2, \tag{50}$$

where η_1 and η_2 are bounded, positive operators with unbounded inverses, the specific form of which depends on the models considered and will be given below. Moreover we assume that there is $\Sigma > \inf \sigma(H_p)$ such that the following estimate holds

$$\|\eta_2^{-n} \eta_1^{-m} \eta_2^{-n} f(H)\| \lesssim 1, \quad 0 \leq n, m \leq 2, \tag{51}$$

for any $f \in \mathrm{C}_0^\infty((-\infty, \Sigma))$.

A primary example for the particle system to have in mind is an electron in a vacuum or in a solid in an external potential V. In this case, $H_p = \epsilon(p) + V(x)$, $p := -i\nabla_x$, with $\epsilon(p)$ being the standard non-relativistic kinetic energy, $\epsilon(p) = \frac{1}{2m}|p|^2 \equiv -\frac{1}{2m}\Delta_x$ (the Nelson model), or the electron dispersion law in a crystal lattice (a standard model in solid state physics), acting on $\mathcal{H}_p = L^2(\mathbb{R}^3)$. The coupling family is given by $g(k) = |k|^\mu \xi(k) e^{ikx}$, where $\xi(k)$ is the ultraviolet cut-off, satisfying e.g. $|\partial^m \xi(k)| \lesssim \langle k \rangle^{-2-\mu}$, $m = 0, \ldots, 3$ (and therefore $g(k)$ satisfies (50), with $\eta_1 = \mathbf{1}$ and $\eta_2 = \langle x \rangle^{-1}$ with $\langle x \rangle = (1 + |x|^2)^{1/2}$). For phonons, $\mu = 1/2$, and for the Nelson model, $\mu \geq -1/2$. To have a self-adjoint operator H we assume that V is a Kato potential and that $\mu \geq -1/2$. This can be easily upgraded to an $N-$body system (e.g. an atom or a molecule, see e.g. [53, 73]).

For the particle models discussed above (both for the non-relativistic QED and phonon models), (51) holds with $\eta_1 = \langle p \rangle^{-1}$ and $\eta_2 = \langle x \rangle^{-1}$.

Spin-boson model Another example fitting into our framework, and one of the simplest one, is the spin-boson model describing an idealized two-level atom, with state space $\mathcal{H}_p = \mathbb{C}^2$ and Hamiltonian $H_p = \varepsilon \sigma^3$, where $\sigma^1, \sigma^2, \sigma^3$ are the usual

2×2 Pauli matrices, and $\varepsilon > 0$ is an atomic energy, interacting with the massless bosonic field. This model is a rather special case of (48)–(49). The total Hamiltonian is given by (48)–(49), with the coupling family given by $g(k) = |k|^{\mu}\xi(k)\sigma^{+}$, $\sigma^{\pm} = \frac{1}{2}(\sigma^{1} \mp i\sigma^{2})$. For the spin-boson model, we can take $\Sigma = \infty$.

Appendix 3: Translationally Invariant Hamiltonians

If we do not assume that the nuclei are infinitely and there are no external forces acting on the system, then the Hamiltonian (3) is translationally symmetric. This leads to conservation of the total momentum (a quantum version of the classical Noether theorem). Indeed, the system of particles interacting with the quantized electromagnetic fields is invariant under translations of the particle coordinates, $\underline{x} \to \underline{x} + \underline{y}$, where $\underline{y} = (y, \dots, y)$ ($n-$ tuple) and the fields, $A(x) \to A(x - y)$, i.e. H commutes with the translations $T_y : \Psi(\underline{x}) \to e^{i\underline{y}\cdot P_{\mathrm{f}}}\Psi(\underline{x} + \underline{y})$, where P_{f} is the momentum operator associated to the quantized radiation field,

$$P_f = \sum_{\lambda} \int dk\, k\, a^{*}_{\lambda}(k) a_{\lambda}(k).$$

It is straightforward to show that T_y are unitary operators and that they satisfy the relations $T_{x+y} = T_x T_y$, and therefore $y \to T_y$ is a unitary Abelian representation of $\mathbb{R}^3$. Finally, we observe that the group T_y is generated by the total momentum operator, P_{tot}, of the electrons and the photon field: $T_y = e^{iy\cdot P_{tot}}$. Here P_{tot} is the selfadjoint operator on $\mathcal{H}$, given by

$$P_{tot} := \sum_i p_i \otimes \mathbf{1}_f + \mathbf{1}_{el} \otimes P_f \tag{52}$$

where, as above, $p_j := -i\nabla_{x_j}$, the momentum of the $j-$th electron and P_f is the field momentum given above. Hence $[H, P_{tot}] = 0$.

Let $\mathcal{H}$ be the direct integral $\mathcal{H} = \int^{\oplus}_{\mathbb{R}^3} \mathcal{H}_P dP$, with the fibers $\mathcal{H}_P := L^2(X) \otimes \mathcal{F}$, where $X := \{x \in \mathbb{R}^{3n} \mid \sum_i m_i x_i = 0\} \simeq \mathbb{R}^{3(n-1)}$, (this means that $\mathcal{H} = L^2(\mathbb{R}^3, dP; L^2(X) \otimes \mathcal{F})$) and define $U : \mathcal{H}_{\mathrm{el}} \otimes \mathcal{H}_{\mathrm{f}} \to \mathcal{H}$ on smooth functions with compact domain by the formula

$$(U\Psi)(\underline{x}', P) = \int_{\mathbb{R}^3} e^{i(P - P_{\mathrm{f}})\cdot x_{cm}} \Psi(\underline{x}' + \underline{x}_{cm}) \mathrm{d}y, \tag{53}$$

where $\underline{x}'$ are the coordinates of the N particles in the center-of-mass frame and $\underline{x}_{cm} = (x_{cm}, \dots, x_{cm})$ ($n-$ tuple), with $x_{cm} = \frac{1}{\sum_i m_i} \sum_i m_i x_i$, the center-of-mass coordinate, so that $\underline{x} = \underline{x}' + \underline{x}_{cm}$. Then U extends uniquely to a unitary operator (see below). Its

converse is written, for $\Phi(\underline{x}', P) \in L^2(X) \otimes \mathcal{F}$, as

$$(U^{-1}\Phi)(\underline{x}) = \int_{\mathbb{R}^3} e^{-ix_{cm}\cdot(P-P_f)}\Phi(\underline{x}', P)\mathrm{d}P. \tag{54}$$

The functions $\Phi(\underline{x}', P) = (U\Psi)(\underline{x}', P)$ are called fibers of Ψ. One can easily prove the following

Lemma 1 *The operations* (53) *and* (54) *define unitary maps* $L^2(\mathbb{R}^{3n}) \otimes \mathcal{F} \to \mathcal{H}$ *and* $\mathcal{H} \to L^2(\mathbb{R}^{3n}) \otimes \mathcal{F}$, *and are mutual inverses.*

Since H commutes with P_{tot}, it follows that it admits the fiber decomposition

$$UHU^{-1} = \int_{\mathbb{R}^3}^{\oplus} H(P)\mathrm{d}P, \tag{55}$$

where the fiber operators $H(P)$, $P \in \mathbb{R}^3$, are self-adjoint operators on $\mathcal{F}$. Using $a(k)e^{-iy\cdot P_f} = e^{-iy\cdot(P_f+k)}a(k)$ and $a^*(k)e^{-iy\cdot P_f} = e^{-iy\cdot(P_f-k)}a^*(k)$, we find $\nabla_y e^{iy\cdot(P-P_f)}A_\xi(x'+y)e^{iy\cdot(P-P_f)} = 0$ and therefore

$$A_\xi(x)e^{iy\cdot(P-P_f)} = e^{iy\cdot(P-P_f)}A_\xi(x-y). \tag{56}$$

Using this and (54), we compute $H(U^{-1}\Phi)(x) = \int_{\mathbb{R}^3} e^{ix\cdot(P-P_f)}H(P)\Phi(P)dP$, where $H(P)$ are Hamiltonians on the space fibers $\mathcal{H}_P := \mathcal{F}$ given explicitly by

$$H(P) = \sum_j \frac{1}{2m_i}\big(P - P_f - i\nabla_{x_j'} - e_i A_\xi(x_j')\big)^2 + V_{\mathrm{coul}}(\underline{x}') + H_f \tag{57}$$

where $x_i' = x_i - x_{cm}$ is the coordinate of the i-th particle in the center-of-mass frame. Now, this Hamiltonian can be investigated similarly to the one in (3).

Appendix 4: Method of Propagation Observables

Many steps of our proof use the method of propagation observables which we formalize in what follows. Let $\psi_t = e^{-itH}\psi_0$, where H is a Hamiltonian of the form (48)–(49), with the coupling operator $g(k)$ satisfying (50) and (51). The method reduces propagation estimates for our system say of the form

$$\int_0^\infty dt \left\| G_t^{\frac{1}{2}}\psi_t \right\|^2 \lesssim \|\psi_0\|_\#^2, \tag{58}$$

for some norm $\|\cdot\|_{\#} \geq \|\cdot\|$, to differential inequalities for certain families ϕ_t of positive, one-photon operators on the one-photon space $L^2(\mathbb{R}^3)$. Let

$$d\phi_t := \partial_t \phi_t + i[\omega, \phi_t].$$

We isolate the following useful class of families of positive, one-photon operators:

Definition 1 A family of positive operators ϕ_t on $L^2(\mathbb{R}^3)$ will be called a *one-photon weak propagation observable*, if it has the following properties

- there are $\delta \geq 0$ and a family p_t of non-negative operators, such that

$$\|\omega^{\delta/2}\phi_t\omega^{\delta/2}\| \lesssim \langle t\rangle^{-\nu_\delta} \quad \text{and} \quad d\phi_t \geq p_t + \sum_{\text{finite}} \text{rem}_i, \tag{59}$$

  where rem_i are one-photon operators satisfying

$$\|\omega^{\rho_i/2}\,\text{rem}_i\,\omega^{\rho_i/2}\| \lesssim \langle t\rangle^{-\lambda_i}, \tag{60}$$

  for some ρ_i and λ_i, s.t. $\lambda_i > 1 + \nu_{\rho_i}$,
- for some $\lambda' > 1 + \nu_\delta$ and with η_1, η_2 satisfying (51),

$$\Big(\int \|\eta_1\eta_2^2(\phi_t g)(k)\|^2_{\mathcal{H}_p}\omega(k)^\delta dk\Big)^{\frac{1}{2}} \lesssim \langle t\rangle^{-\lambda'}. \tag{61}$$

  (Here ϕ_t acts on g as a function of k.)

Similarly, a family of operators ϕ_t on $L^2(\mathbb{R}^3)$ will be called a *one-photon strong propagation observable*, if

$$d\phi_t \leq -p_t + \sum_{\text{finite}} \text{rem}_i, \tag{62}$$

with $p_t \geq 0$, rem_i are one-photon operators satisfying (60) for some $\lambda_i > 1 + \nu_{\rho_i}$, and (61) holds for some $\lambda' > 1 + \nu_\delta$.

The following proposition reduces proving inequalities of the type of (58) to showing that ϕ_t is a one-photon weak or strong propagation observable, i.e. to *one-photon estimates* of $d\phi_t$ and $\phi_t g$.

Proposition 1 *If ϕ_t is a one-photon weak (resp. strong) propagation observable, then we have either the weak propagation estimate, (58), or the strong propagation estimate,*

$$\langle\psi_t, \Phi_t\psi_t\rangle + \int_0^\infty dt\,\big\|G_t^{\frac{1}{2}}\psi_t\big\|^2 \lesssim \|\psi_0\|^2_{\#}, \tag{63}$$

with the norm $\|\psi_0\|_{\#}^2 := \|\psi_0\|_{\diamond}^2 + \|\psi_0\|_*^2$, *where* $\Phi_t := \mathrm{d}\Gamma(\phi_t)$, $G_t := \mathrm{d}\Gamma(p_t)$, $\|\psi_0\|_* := \|\psi_0\|_\delta$ *and* $\|\psi_0\|_\diamond := \sum \|\psi_0\|_{\rho_i}$, *on the subspace* $\Upsilon_{\max(\delta,\rho_i)}$.

Before proceeding to the proof we present some useful definitions. Consider families Φ_t of operators on $\mathcal{H}$ and introduce the Heisenberg derivative

$$D\Phi_t := \partial_t \Phi_t + i\big[H, \Phi_t\big],$$

with the property

$$\partial_t \langle \psi_t, \Phi_t \psi_t \rangle = \langle \psi_t, D\Phi_t \psi_t \rangle. \tag{64}$$

Definition 2 A family of self-adjoint operators Φ_t on a subspace $\mathcal{H}_1 \subset \mathcal{H}$ will be called a (second quantized) *weak propagation observable*, if for all $\psi_0 \in \mathcal{H}_1$, it has the following properties

- $\sup_t \langle \psi_t, \Phi_t \psi_t \rangle \lesssim \|\psi_0\|_*^2$;
- $D\Phi_t \geq G_t + \mathrm{Rem}$, where $G_t \geq 0$ and $\int_0^\infty dt\, |\langle \psi_t, \mathrm{Rem}\, \psi_t \rangle| \lesssim \|\psi_0\|_\diamond^2$,

for some norms $\|\psi_0\|_*$, $\|\cdot\|_\diamond \geq \|\cdot\|$. Similarly, a family of operators Φ_t will be called a *strong propagation observable*, if it has the following properties

- Φ_t is a family of non-negative operators;
- $D\Phi_t \leq -G_t + \mathrm{Rem}$, where $G_t \geq 0$ and $\int_0^\infty dt\, |\langle \psi_t, \mathrm{Rem}\, \psi_t \rangle| \lesssim \|\psi_0\|_{\#}^2$,

for some norm $\|\cdot\|_\# \geq \|\cdot\|$.

If Φ_t is a weak propagation observable, then integrating the corresponding differential inequality sandwiched by ψ_t's and using the estimate on $\langle \psi_t, \Phi_t \psi_t \rangle$ and on the remainder Rem, we obtain the (weak propagation) estimate (58), with $\|\psi_0\|_{\#}^2 := \|\psi_0\|_{\diamond}^2 + \|\psi_0\|_*^2$. If Φ_t is a strong propagation observable, then the same procedure leads to the (strong propagation) estimate (63).

Proof of Proposition 1. Let $\Phi_t := \mathrm{d}\Gamma(\phi_t)$. To prove the above statement we use the relations (see Supplement II)

$$D_0 \mathrm{d}\Gamma(\phi_t) = \mathrm{d}\Gamma(d\phi_t), \qquad i[I(g), \mathrm{d}\Gamma(\phi_t)] = -I(i\phi_t g), \tag{65}$$

where D_0 is the free Heisenberg derivative,

$$D_0 \Phi_t := \partial_t \Phi_t + i[H_0, \Phi_t],$$

valid for any family of one-particle operators ϕ_t, to compute

$$D\Phi_t = \mathrm{d}\Gamma(d\phi_t) - I(i\phi_t g). \tag{66}$$

Denote $\langle A\rangle_\psi := \langle\psi, A\psi\rangle$. Applying the Cauchy-Schwarz inequality, we find the following version of a standard estimate

$$|\langle I(g)\rangle_\psi| \le 2\Big(\int \|\eta_1\eta_2^2 g(k)\|^2_{\mathcal{H}_p}\omega(k)^\delta d^3k\Big)^{\frac{1}{2}} \|\eta_1^{-1}\eta_2^{-2}\psi\|\|\psi\|_\delta. \tag{67}$$

Using that $\psi_t = f_1(H)\psi_t$, with $f_1 \in C_0^\infty((-\infty, \Sigma))$, $f_1 f = f$, and using (51), we find $\|\eta_1^{-1}\eta_2^{-2}\psi_t\| \lesssim \|\psi_t\|$. Taking this into account, we see that the Eqs. (67), (61) and $\|\psi_t\|_{H_f} \lesssim \|\psi_0\|_H$ yield

$$|\langle I(i\phi_t g)\rangle_{\psi_t}| \lesssim \langle t\rangle^{-\lambda'+\nu_\delta}\|\psi_0\|^2_\delta. \tag{68}$$

Next, using (60), we find $\pm\mathrm{rem}_i \le \|\omega^{\rho_i/2}\,\mathrm{rem}_i\,\omega^{\rho_i/2}\|\omega^{\rho_i} \lesssim \langle t\rangle^{-\lambda_i}\omega^{-\rho_i}$. This gives $\pm\mathrm{d}\Gamma(\mathrm{rem_i}) \lesssim \langle t\rangle^{-\lambda_i}\mathrm{d}\Gamma(\omega^{-\rho_i})$, which, due to the bound (22), leads to the estimate

$$\big|\langle \mathrm{d}\Gamma(\mathrm{rem_i})\rangle_{\psi_t}\big| \lesssim \langle t\rangle^{-\lambda_i+\nu_{\rho_i}}\|\psi_0\|^2_{\rho_i}. \tag{69}$$

Let $G_t := \mathrm{d}\Gamma(p_t)$ and $\mathrm{Rem} := \sum_{\mathrm{finite}}\mathrm{d}\Gamma(\mathrm{rem_i}) - I(i\phi_t g)$. We have $G_t \ge 0$, and, by (68) and (69),

$$\int_0^\infty dt\,\big|\langle\psi_t, \mathrm{Rem}\,\psi_t\rangle\big| \lesssim \|\psi_0\|^2_\diamond, \tag{70}$$

with $\|\psi_0\|^2_\# := \|\psi_0\|^2_\diamond + \|\psi_0\|^2_*$, $\|\psi_0\|_* := \|\psi_0\|_\delta$, $\|\psi_0\|_\diamond := \sum\|\psi_0\|_{\rho_i}$.

In the strong case, (62) and (66) imply

$$D\Phi_t \le -G_t + \mathrm{Rem}, \tag{71}$$

and hence by (70), Φ_t is a strong propagation observable.

In the weak case, (59) and (66) imply

$$D\Phi_t \ge G_t + \mathrm{Rem}. \tag{72}$$

Since $\phi_t \le \|\omega^{\delta/2}\phi_t\omega^{\delta/2}\|\omega^{-\delta} \lesssim \langle t\rangle^{-\nu_\delta}\omega^{-\delta}$, we have $\mathrm{d}\Gamma(\phi_t) \lesssim \langle t\rangle^{-\nu_\delta}\mathrm{d}\Gamma(\omega^{-\delta})$. Using this estimate and using again the bound (22), we obtain

$$\langle\psi_t, \Phi_t\psi_t\rangle \lesssim \langle t\rangle^{-\nu_\delta}\langle\mathrm{d}\Gamma(\omega^{-\delta})\rangle_{\psi_t} \lesssim \|\psi_0\|^2_\delta. \tag{73}$$

Estimates (70) and (73) show that Φ_t is a weak propagation observable. □

Remark Proposition 1 reduces a proof of propagation estimates for the dynamics (1) to estimates involving the *one-photon* datum (ω, g) (an 'effective one-photon system'), parameterizing the Hamiltonian (48). (The remaining datum H_p does not

enter our analysis explicitly, but through the bound states of H_p which lead to the localization in the particle variables, (51)).

To prove the first propagation estimate (Theorem 4.1), we use the method of propagation observables outlined above. We consider the one-parameter family of one-photon operators

$$\phi_t := t^{-av_0}\chi_\alpha, \quad \chi_\alpha \equiv \chi_{v\geq 1}, \quad v := \frac{b_\epsilon}{ct^\alpha}, \tag{74}$$

where $a > 1$ and recall the operator b_ϵ defined in Sect. 4. We use the fact that commutators of two $\mathrm{d}\Gamma$ operators reduces to commutators of the one-particle operators:

$$[\mathrm{d}\Gamma(\tau), \mathrm{d}\Gamma(\tau')] = \mathrm{d}\Gamma([\tau, \tau']). \tag{75}$$

For the second estimate (Theorem 4.2), we use the propagation observable

$$\Phi_t := -t^\rho \varphi\big(B_{\epsilon,t}\big),$$

where $B_{\epsilon,t} := B_\epsilon/(ct)$, with $B_\epsilon := \mathrm{d}\Gamma(b_\epsilon)$, and $\varphi\big(B_{\epsilon,t}\big) := \big(B_{\epsilon,t} - 2\big)\chi_{B_{\epsilon,t}\leq 1}$. Note that $\varphi \leq 0$, but $\varphi' \geq 0$.

Appendix 5: Local Decay

For any compactly supported function $f(\lambda)$ with $\mathrm{supp} f \subseteq (\inf H, \infty)/(\text{a neighbourhood of } \Sigma)$, and for $\theta > \frac{1}{2}$, $\nu < \theta - \frac{1}{2}$, we have that

$$\|\langle Y\rangle^{-\theta} e^{-iHt} f(H) \langle Y\rangle^{-\theta}\| \leq Ct^{-\nu}. \tag{76}$$

Here $\langle Y\rangle := (\mathbf{1} + Y^2)^{1/2}$, and Y denotes the self-adjoint operator on Fock space $\mathcal{F}$ of photon co-ordinate,

$$Y := \int d^3k\, a^*(k)\, i\nabla_k\, a(k), \tag{77}$$

extended to the Hilbert space $\mathcal{H} = \mathcal{H}_p \otimes \mathcal{F}$. (A self-adjoint operator H obeying (76) is said to have the (Δ, ν, Y, θ) - *local decay* (LD) property.) (76) shows that for well-prepared initial conditions ψ_0, the probability of finding photons within a ball of an arbitrary radius $R < \infty$, centered say at the center-of-mass of the particle system, tends to 0, as time t tends to ∞.

Note that one can also show that as $t \to \infty$, the photon coordinate and wave vectors in the support of the solution $e^{-iHt}\psi_0$ of the Schrödinger equation become

more and more parallel. This follows from the local decay for the self-adjoint generator of dilatations on Fock space $\mathcal{F}$,

$$B := \frac{i}{2} \int d^3k \, a^*(k) \left\{ k \cdot \nabla_k + \nabla_k \cdot k \right\} a(k). \tag{78}$$

(In fact, one first proves the local decay property for B and then transfers it to the photon co-ordinate operator Y.)

Appendix 6: Supplement: Creation and Annihilation Operators

Recall that the propagation speed of the light and the Planck constant divided by 2π are set equal to 1 and that the one-particle space is $\mathfrak{h} := \mathrm{L}^2(\mathbb{R}^3; \mathbb{C})$, for phonons, and $\mathfrak{h} := \mathrm{L}^2(\mathbb{R}^3; \mathbb{C}^2)$, for photons. In both cases we use the momentum representation and write functions from this space as $u(k)$ and $u(k, \lambda)$, respectively, where $k \in \mathbb{R}^3$ is the wave vector or momentum of the photon and $\lambda \in \{-1, +1\}$ is its polarization. The Bosonic Fock space, $\mathcal{F}$, over $\mathfrak{h}$ is defined by

$$\mathcal{F} := \bigoplus_{n=0}^{\infty} \mathcal{S}_n \, \mathfrak{h}^{\otimes n},$$

where $\mathcal{S}_n$ is the orthogonal projection onto the subspace of totally symmetric n-particle wave functions contained in the n-fold tensor product $\mathfrak{h}^{\otimes n}$ of $\mathfrak{h}$; and

$$\mathcal{S}_0 \mathfrak{h}^{\otimes 0} := \mathbb{C}.$$

The vector $\Omega := (1, 0, \ldots)$ is called the *vacuum vector* in $\mathcal{F}$. Vectors $\Psi \in \mathcal{F}$ can be identified with sequences $(\psi_n)_{n=0}^{\infty}$ of n-particle wave functions, which are totally symmetric in their n arguments, and $\psi_0 \in \mathbb{C}$. In the first case these functions are of the form, $\psi_n(k_1, \ldots, k_n)$, while in the second case, of the form $\psi_n(k_1, \lambda_1, \ldots, k_n, \lambda_n)$, where $\lambda_j \in \{-1, 1\}$ are the polarization variables.

In what follows we present some key definitions in the first case, limiting ourselves to remarks at the end of this appendix on how these definitions have to be modified for the second case. The scalar product of two vectors Ψ and Φ is given by

$$\langle \Psi \, , \, \Phi \rangle := \sum_{n=0}^{\infty} \int \prod_{j=1}^{n} d^3k_j \, \overline{\psi_n(k_1, \ldots, k_n)} \, \varphi_n(k_1, \ldots, k_n).$$

Given a one particle dispersion relation $\omega(k)$, the energy of a configuration of n *non-interacting* field particles with wave vectors $k_1, \ldots, k_n$ is given by $\sum_{j=1}^{n} \omega(k_j)$.

We define the *free-field Hamiltonian*, H_f, giving the field dynamics, by

$$(H_f\Psi)_n(k_1,\ldots,k_n) \;=\; \Big(\sum_{j=1}^{n}\omega(k_j)\Big)\,\psi_n(k_1,\ldots,k_n),$$

for $n \geq 1$ and $(H_f\Psi)_n = 0$ for $n = 0$. Here $\Psi = (\psi_n)_{n=0}^{\infty}$ (to be sure that the r.h.s. makes sense we can assume that $\psi_n = 0$, except for finitely many n, for which $\psi_n(k_1,\ldots,k_n)$ decrease rapidly at infinity). Clearly that the operator H_f has the single eigenvalue 0 with the eigenvector Ω and the rest of the spectrum absolutely continuous.

With each function $f \in \mathfrak{h}$, one associates *creation* and *annihilation operators* $a(f)$ and $a^*(f)$ defined, for $u \in \otimes_s^n\mathfrak{h}$, as

$$a^*(f) : u \to \sqrt{n+1}f \otimes_s u \quad \text{and} \quad a(f) : u \to \sqrt{n}\langle f, u\rangle_{\mathfrak{h}},$$

with $\langle f,u\rangle_{\mathfrak{h}} := \int \overline{f(k)}u(k,k_1,\ldots,k_{n-1})\,\mathrm{d}k$, for phonons, and $\langle f,u\rangle_{\mathfrak{h}} := \sum_{\lambda=1,2}\int \mathrm{d}k\overline{f(k,\lambda)}u_n(k,\lambda,k_1,\lambda_1,\ldots,k_{n-1},\lambda_{n-1})$, for photons. They are unbounded, densely defined operators of $\Gamma(\mathfrak{h})$, adjoint of each other (with respect to the natural scalar product in $\mathcal{F}$) and satisfy the *canonical commutation relations* (CCR):

$$\big[a^{\#}(f), a^{\#}(g)\big] = 0, \qquad \big[a(f), a^*(g)\big] = \langle f, g\rangle,$$

where $a^{\#} = a$ or a^*. Since $a(f)$ is anti-linear and $a^*(f)$ is linear in f, we write formally, for photons,

$$a(f) = \sum_{\lambda=1,2}\int \overline{f(k,\lambda)}a_\lambda(k)\,dk, \qquad a^*(f) = \sum_{\lambda=1,2}\int f(k,\lambda)a_\lambda^*(k)dk.$$

Here $a_\lambda(k)$ and $a_\lambda^*(k)$ are unbounded, operator-valued distributions, which obey (again formally) the *canonical commutation relations* (CCR):

$$\big[a_\lambda^{\#}(k), a_{\lambda'}^{\#}(k')\big] = 0, \qquad \big[a_\lambda(k), a_{\lambda'}^*(k')\big] = \delta_{\lambda,\lambda'}\delta(k-k'),$$

where $a_\lambda^{\#} = a_\lambda$ or a_λ^*.

Given an operator τ acting on the one-particle space $\mathfrak{h}$, the operator $\mathrm{d}\Gamma(\tau)$ (the second quantization of τ) defined on the Fock space $\mathcal{F}$ by (15), can be written (formally), for photons, as $\mathrm{d}\Gamma(\tau) := \sum_{\lambda=1,2}\int dk\, a_\lambda^*(k)\tau a_\lambda(k)$. Here the operator τ acts on the k-variable. The precise meaning of the latter expression is (15). In particular, one can rewrite the quantum Hamiltonian H_f in terms of the creation and annihilation operators, a and a^*, as

$$H_f = \sum_{\lambda=1,2}\int dk\, a_\lambda^*(k)\omega(k)a_\lambda(k).$$

More generally, for any operator, t, on the one-particle space $L^2(\mathbb{R}^3, \mathbb{C}, d^3k)$ we define the operator T on the Fock space $\mathcal{F}$ by the following formal expression $T := \int a^*(k)ta(k)dk$, where the operator t acts on the $k-$variable (T is the second quantization of t). The precise meaning of the latter expression can obtained by using a basis $\{\phi_j\}$ in the space $L^2(\mathbb{R}^3, \mathbb{C}, d^3k)$ to rewrite it as $T := \sum_j \int a^*(\phi_j)a(t^*\phi_j)dk$.

One can introduce the operator-valued transverse vector fields by

$$a^{\#}(k) := \sum_{\lambda\in\{-1,1\}} e_\lambda(k)a^{\#}_\lambda(k),$$

where $e_\lambda(k) \equiv e(k,\lambda)$ are polarization vectors, i.e., orthonormal vectors in $\mathbb{R}^3$ satisfying $k \cdot e_\lambda(k) = 0$.

For phonons, the expressions are simpler. For instance, we can write $a^{\#}(f)$ formally as

$$a(f) = \int \overline{f(k)}a(k)\,dk, \qquad a^*(f) = \int f(k)a^*(k)\,dk,$$

with unbounded, operator-valued distributions, $a(k)$ and $a^*(k)$ obeying (again formally) the *canonical commutation relations* (CCR):

$$\left[a^{\#}(k), a^{\#}(k')\right] = 0, \qquad \left[a(k), a^*(k')\right] = \delta(k-k'),$$

where $a^{\#} = a$ or a^*.

Acknowledgements The author is grateful to Walid Abou Salem, Thomas Chen, Jérémy Faupin, Marcel Griesemer and especially Volker Bach and Jürg Fröhlich, and Avy Soffer for fruitful collaboration and for all they have taught him in the course of joint work.

References

1. W. Amrein, Localizability for particles of mass zero. Helv. Phys. Acta **42**, 149–190 (1969)
2. A. Arai, A note on scattering theory in nonrelativistic quantum electrodynamics. J. Phys. A **16**, 49–69 (1983)
3. A. Arai, Long-time behavior of an electron interacting with a quantized radiation field. J. Math. Phys. **32**, 2224–2242 (1991)
4. V. Bach, Mass renormalization in nonrelativisitic quantum electrodynamics, in *Quantum Theory from Small to Large Scales*. Lecture Notes of the Les Houches Summer Schools, vol. 95 (Oxford University Press, 2011)
5. V. Bach, T. Chen, J. Fröhlich, I.M. Sigal, Smooth Feshbach map and operator-theoretic renormalization group methods. J. Funct. Anal. **203**, 44–92 (2003)
6. V. Bach, T. Chen, J. Fröhlich, I.M. Sigal, The renormalized electron mass in non-relativistic quantum electrodynamics. J. Funct. Anal. **243**, 426–535 (2007)
7. V. Bach, J. Fröhlich, I.M. Sigal, Quantum electrodynamics of confined non-relativistic particles. Adv. Math. **137**, 205–298; 299–395 (1998)

8. V. Bach, J. Fröhlich, I.M. Sigal, Spectral analysis for systems of atoms and molecules coupled to the quantized radiation field. Commun. Math. Phys. **207**, 249–290 (1999)
9. V. Bach, J. Fröhlich, I.M. Sigal, A. Soffer, Positive commutators and spectrum of Pauli-Fierz Hamiltonian of atoms and molecules. Commun. Math. Phys. **207**, 557–587 (1999)
10. J.-F. Bony, J. Faupin, Resolvent smoothness and local decay at low energies for the standard model of non-relativistic QED. J. Funct. Anal. **262**, 850–888 (2012)
11. J.-F. Bony, J. Faupin, I.M. Sigal, Maximal velocity of photons in non-relativistic QED. Adv. Math. **231**, 3054–3078 (2012)
12. D. Buchholz, Collision theory for massless bosons. Comm. Math. Phys. **52**, 147–173 (1977)
13. T. Chen, J. Faupin, J. Fröhlich, I.M. Sigal, Local decay in non-relativistic QED. Commun. Math. Phys. **309**, 543–583 (2012)
14. T. Chen, Infrared renormalization in non-relativistic QED and scaling criticality. J. Funct. Anal. **254**, 2555–2647 (2008)
15. T. Chen, J. Fröhlich, Coherent infrared representations in non-relativistic QED, in *Spectral Theory and Mathematical Physics: A Festschrift in Honor of Barry Simon's 60th Birthday.* Proceedings of Symposia in Pure Mathematics (AMS, Providence, 2007)
16. T. Chen, J. Fröhlich, A. Pizzo, Infraparticle scattering states in non-relativistic QED – I. The Bloch-Nordsieck paradigm. Commun. Math. Phys. **294**, 761–825 (2010)
17. T. Chen, J. Fröhlich, A. Pizzo, Infraparticle scattering states in non-relativistic QED – II. Mass shell properties. J. Math. Phys. **50**, 012103 34 (2009)
18. C. Cohen-Tannoudji, J. Dupont-Roc, G. Grynberg, *Photons and Atoms: Introduction to Quantum Electrodynamics.* Wiley Professional Paperback Series (Wiley, New York, 1997)
19. C. Cohen-Tannoudji, J. Dupont-Roc, G. Grynberg, *Atom-Photon Interactions – Basic Processes and Applications* (John Wiley, New York, 1992)
20. W. De Roeck, A. Kupiainen, Approach to ground state and time-independent photon bound for massless spin-boson models. Ann. Henri Poincaré **14**, 253–311 (2013)
21. W. De Roeck, M. Griesemer, A. Kupiainen, Asymptotic completeness for the massless spin-boson model. Adv. Math. **268**, 62–84 (2015)
22. P. Deift, B. Simon, A time-dependent approach to the completeness of multiparticle quantum systems. Comm. Pure Appl. Math. **30**, 573–583 (1977)
23. J. Dereziński, Asymptotic completeness of long-range N-body quantum systems. Ann. Math. **138**, 427–476 (1993)
24. J. Dereziński, *Bogolubov Transformations.* Accessed Aug 2014. Available at: http://www.fuw.edu.pl/~derezins/bogo-slides.pdf
25. J. Dereziński, C. Gérard, *Scattering Theory of Classical and Quantum N-Particle Systems.* Texts and Monographs in Physics (Springer, Berlin/New York, 1997)
26. J. Dereziński, C. Gérard, Asymptotic completeness in quantum field theory. Massive Pauli-Fierz Hamiltonians. Rev. Math. Phys. **11**, 383–450 (1999)
27. J. Dereziński, C. Gérard, Spectral and scattering theory of spatially cut-off $P(\varphi)_2$ Hamiltonians. Comm. Math. Phys. **213**, 39–125 (2000)
28. J. Dereziński, C. Gérard, *Mathematics of Quantization and Quantum Fields.* Cambridge Monographs in Mathematical Physics (Cambridge University Press, Cambridge, 2013)
29. W. Dybalski, Asymptotic observables, propagation estimates and the problem of asymptotic completeness in algebraic QFT, in *Contribution to Proceedings of QMath12*. http://arxiv.org/abs/1402.6549
30. W. Dybalski, Ch. Gérard, *A Criterion for Asymptotic Completeness in Local Relativistic QFT.* arXiv:1308.5187
31. W. Dybalski, A. Pizzo, *Coulomb Scattering in the Massless Nelson Model II. Regularity of Ground States.* arXiv:1302.5012
32. W. Dybalski, A. Pizzo, *Coulomb Scattering in the Massless Nelson Model I. Foundations of Two-Electron Scattering.* arXiv:1302.5001
33. W. Dybalski, Ch. Gérard, *Towards Asymptotic Completeness of Two-Particle Scattering in Local Relativistic QFT.* arXiv:1211.3393

34. W. Dybalski, J.S. Møller, *The Translation Invariant Massive Nelson Model: III. Asymptotic Completeness Below the Two-Boson Threshold.* arXiv:1210.6645
35. J. Faupin, I.M. Sigal, On Rayleigh scattering in non-relativistic quantum electrodynamics. Comm. Math. Phys. **328**, 1199–1254 (2014)
36. J. Faupin, I.M. Sigal, Minimal photon velocity bounds in non-relativistic quantum electrodynamics. J. Stat. Phys. **154**, 58–90 (2014)
37. E. Fermi, Quantum theory of radiation. Rev. Mod. Phys. **4**, 87–132 (1932)
38. J. Fröhlich, On the infrared problem in a model of scalar electrons and massless, scalar bosons. Ann. Inst. Henri Poincaré **19**, 1–103 (1973)
39. J. Fröhlich, Existence of dressed one electron states in a class of persistent models. Fortschr. Phys. **22**, 159–198 (1974)
40. J. Fröhlich, M. Griesemer, B. Schlein, Asymptotic electromagnetic fields in models of quantum-mechanical matter interacting with the quantized radiation field. Adv. Math. **164**, 349–398 (2001)
41. J. Fröhlich, M. Griesemer, B. Schlein, Asymptotic completeness for Rayleigh scattering. Ann. Henri Poincaré **3** (2002) 107–170.
42. J. Fröhlich, M. Griesemer, B. Schlein, Asymptotic completeness for Compton scattering. Comm. Math. Phys. **252**, 415–476 (2004)
43. J. Fröhlich, M. Griesemer, B. Schlein, Rayleigh scattering at atoms with dynamical nuclei. Comm. Math. Phys. **271**, 387–430 (2007)
44. J. Fröhlich, M. Griesemer, I.M. Sigal, Spectral theory for the standard model of non-relativisitc QED. Comm. Math. Phys. **283**, 613–646 (2008)
45. J. Fröhlich, M. Griesemer, I.M. Sigal, Spectral renormalization group and limiting absorption principle for the standard model of non-relativisitc QED. Rev. Math. Phys. **23**, 179–209 (2011)
46. V. Georgescu, C. Gérard, J.S. Møller, Commutators, C_0-semigroups and resolvent estimates. J. Funct. Anal. **216**, 303–361 (2004)
47. V. Georgescu, C. Gérard, J.S. Møller, Spectral theory of massless Pauli-Fierz models. Comm. Math. Phys. **249**, 29–78 (2004)
48. C. Gérard, On the scattering theory of massless Nelson models. Rev. Math. Phys. **14**, 1165–1280 (2002)
49. G.-M. Graf, D. Schenker, Classical action and quantum *N*-body asymptotic completeness, in *Multiparticle Quantum Scattering with Applications to Nuclear, Atomic and Molecular Physics (1995)*, Minneapolis (Springer, New York, 1997), pp. 103–119
50. M. Griesemer, Exponential decay and ionization thresholds in non-relativistic quantum electrodynamics. J. Funct. Anal. **210**, 321–340 (2004)
51. M. Griesemer, E.H. Lieb, M. Loss, Ground states in non-relativistic quantum electrodynamics. Invent. Math. **145**, 557–595 (2001)
52. M. Griesemer, H. Zenk, Asymptotic electromagnetic fields in non-relativistic QED: the problem of existence revisited. J. Math. Anal. Appl. **354**, 239–246 (2009)
53. S. Gustafson, I.M. Sigal, *Mathematical Concepts of Quantum Mechanics*. Universitext, 2nd edn. (Springer, Berlin/Heidelberg, 2011)
54. D. Hasler, I. Herbst, On the self-adjointness and domain of Pauli–Fierz type Hamiltonians. Rev. Math. Phys. **20**, 787–800 (2008)
55. F. Hiroshima, Self-adjointness of the Pauli–Fierz Hamiltonian for arbitrary values of coupling constants. Ann. Henri Poincaré **3**, 171–201 (2002)
56. M. Hübner, H. Spohn, Radiative decay: nonperturbative approaches. Rev. Math. Phys. **7**, 363–387 (1995)
57. W. Hunziker, I.M. Sigal, The quantum *N*-body problem. J. Math. Phys. **41**, 3448–3510 (2000)
58. W. Hunziker, I.M. Sigal, A. Soffer, Minimal escape velocities. Comm. Partial Differ. Eqns. **24**, 2279–2295 (1999)
59. J.M. Jauch, C. Piron, Generalized localizability. Helv. Phys. Acta **40**, 559–570 (1967)
60. O. Keller, On the theory of spatial localization of photons. Phys. Rep. **411**, 1–232 (2005)
61. Ch. Kittel, *Quantum Theory of Solids*, 2nd edn. (Wiley, New York, 1987)

62. L. Landau, R. Peierls, Quantenelektrodynamik im Konfigurationsraum. Z. Phys. **62**, 188–200 (1930)
63. E. Lieb, M. Loss, Existence of atoms and molecules in non-relativistic quantum electrodynamics. Adv. Theor. Math. Phys. **7**, 667–710 (2003)
64. E. Lieb, M. Loss, A note on polarization vectors in quantum electrodynamics. Comm. Math. Phys. **252**, 477–483 (2004)
65. L. Mandel, Configuration-space photon number operators in quantum optics. Phys. Rev. **144**, 1071–1077 (1966)
66. L. Mandel, E. Wolf, *Optical Coherence and Quantum Optics* (Cambridge University Press, Cambridge/New York, 1995)
67. T.D. Newton, E. Wigner, Localized states for elementary systems. Rev. Mod. Phys. **21**, 400–406 (1949)
68. W. Pauli, *Collected Scientific Papers*, vol. 2 (Interscience Publishers, New York, 1964)
69. W. Pauli, M. Fierz, Zur Theorie der Emission langwelliger Lichtquanten. Il Nuovo Cimento **15**, 167–188 (1938)
70. S. Ruijsenaars, On Newton–Wigner localization and superluminal propagation speeds. Ann. Phys. **137**, 33–43 (1981)
71. J.J. Sakurai, *Advanced Quantum Mechanics* (Addison-Wesley, Redwood City, 1987)
72. I.M. Sigal, Ground state and resonances in the standard model of the non-relativistic QED. J. Stat. Phys. **134**, 899–939 (2009)
73. I.M. Sigal, Renormalization group and problem of radiation, in *Lecture Notes of Les Houches Summer School on "Quantum Theory From Small to Large Scales"*, vol. 95 (2012). arXiv. :1110.3841
74. I.M. Sigal, A. Soffer, The *N*-particle scattering problem: asymptotic completeness for short-range quantum systems. Ann. Math. **125**, 35–108 (1987)
75. I.M. Sigal, A. Soffer, Local decay and propagation estimates for time dependent and time independent Hamiltonians (Princeton University, 1988). Preprint
76. I.M. Sigal, A. Soffer, Long-range many-body scattering. Asymptotic clustering for Coulomb-type potentials. Invent. Math. **99**, 115–143 (1990)
77. E. Skibsted, Spectral analysis of *N*-body systems coupled to a bosonic field. Rev. Math. Phys. **10**, 989–1026 (1998)
78. H. Spohn, Asymptotic completeness for Rayleigh scattering. J. Math. Phys. **38**, 2281–2288 (1997)
79. H. Spohn, *Dynamics of Charged Particles and Their Radiation Field* (Cambridge University Press, Cambridge, 2004)
80. A. Wightman, On the localizibility of quantum mechanical systems. Rev. Mod. Phys. **34**, 845–872 (1962)
81. D. Yafaev, Radiation conditions and scattering theory for *N*-particle Hamiltonians. Comm. Math. Phys. **154**, 523–554 (1993)

Avoiding Ultraviolet Divergence by Means of Interior–Boundary Conditions

Stefan Teufel and Roderich Tumulka

Contents

We are grateful to our collaborators Jonas Lampart and Julian Schmidt for their help in developing this approach. We also thank Klaus Fredenhagen, Sheldon Goldstein, Harald Grosse, Stefan Keppeler, and Michael Kiessling for helpful discussions. R.T. was supported in part by grant no. 37433 from the John Templeton Foundation.

S. Teufel (✉)
Mathematisches Institut, Eberhard-Karls-Universität, Auf der Morgenstelle 10, 72076 Tübingen, Germany
e-mail: stefan.teufel@uni-tuebingen.de

R. Tumulka
Department of Mathematics, Rutgers University, 110 Frelinghuysen Road, Piscataway, NJ 08854-8019, USA
e-mail: tumulka@math.rutgers.edu

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_14

Abstract We describe here a novel way of defining Hamiltonians for quantum field theories (QFTs), based on the particle–position representation of the state vector and involving a condition on the state vector that we call an "interior–boundary condition." At least for some QFTs (and, we hope, for many), this approach leads to a well-defined, self-adjoint Hamiltonian without the need for an ultraviolet cut-off or renormalization.

Keywords Regularization of quantum field theory • Ultraviolet infinity • Particle creation and annihilation • Self-adjointness • Schrödinger operator • Boundary condition

Mathematics Subject Classification (2010). 81T10, 81Q10, 35F16, 35Q41

1 Introduction

In quantum field theories (QFTs), the terms in the Hamiltonian governing particle creation and annihilation are usually ultraviolet (UV) divergent. The problem can be circumvented by a UV cut-off, that is, by either discretizing space or attributing a nonzero radius to the electron (or other particles). Another, novel approach [10, 19] is outlined here, leading to Hamiltonians that are well defined, involve particle creation and annihilation, treat space as a continuum, and give radius zero to electrons. They are defined in the particle-position representation of Fock space by means of a new kind of boundary condition on the wave function, which we call an *interior-boundary condition* (IBC) because it relates values of the wave function on a boundary of configuration space to values in the interior. Here, the relevant configuration space is that of a variable number of particles, the relevant boundary consists of the collision configurations (i.e., those at which two or more particles meet), and the relevant interior point lies in a sector with fewer particles.

An IBC is a rather simple condition and provides, as we explain below, a mathematically natural way of implementing particle creation and annihilation at a source of radius zero. It is associated with a Hamiltonian H_{IBC} defined on a domain consisting of functions that satisfy the IBC. For several models that our collaborators Jonas Lampart, Julian Schmidt, and we have studied, we have been able to prove the self-adjointness of H_{IBC}; these results ensure that H_{IBC} is free of divergence problems, UV or otherwise. For suitable choice of the IBC, the Hamiltonian also seems physically plausible, for several reasons that we will describe in more detail in Sect. 4: (i) H_{IBC} has relevant similarities to the original, UV divergent expression for H that one would guess from physical principles; these similarities make H_{IBC} seem like a natural interpretation of that expression. (ii) H_{IBC} has properties and consequences that seem physically reasonable. (iii) In certain models it is possible, after starting from the original expression for H and introducing a UV cut-off, to obtain a well-defined limiting Hamiltonian H_∞ by taking a suitable limit of

removing the cut-off; H_∞ is called a renormalized Hamiltonian (see, e.g., [6]). We have found in such cases that H_{IBC} agrees with H_∞ up to addition of a finite constant; this result supports that H_{IBC} is physically reasonable and, conversely, provides an explicit description of H_∞ that was not available so far.

In this paper, we focus on *non-relativistic* Hamiltonians; there is work in progress [12] about similar constructions with the Dirac operator. Further work on IBCs is forthcoming in [7, 9, 11]. A future goal is to formulate quantum electrodynamics (QED) in terms of IBCs, building particularly on the work of Landau and Peierls [13] about QED in the particle-position representation.

This paper is organized as follows. In Sect. 2, we give a gentle introduction to the idea of an interior–boundary condition by means of a toy quantum theory. In Sect. 3, we describe a similar IBC and Hamiltonian involving particle creation and annihilation. In Sect. 4, we describe how this can be applied to QFTs by means of the particle-position representation, and report some results on the rigorous existence of self-adjoint Hamiltonians defined by means of IBCs.

2 Simple Example of an Interior–Boundary Condition

To introduce the concept of an IBC, we start with a toy example, for which we will set up a "configuration space" $\mathcal{Q}$, a Hilbert space $\mathscr{H} = L^2(\mathcal{Q})$, and a Hamiltonian H on $\mathscr{H}$.

2.1 Configuration Space and Hilbert Space

Consider, as the configuration space $\mathcal{Q}$, the (disjoint) union of $\mathcal{Q}^{(1)} = \mathbb{R}$ and $\mathcal{Q}^{(2)} = \{(x, y) \in \mathbb{R}^2 : y \geq 0\}$; see Fig. 1.

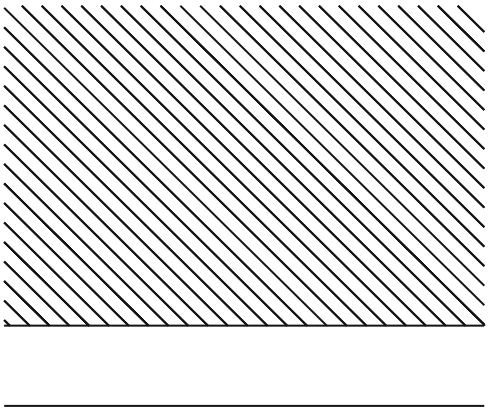


Fig. 1 The configuration space of the toy example consists of two disconnected parts of different dimensions, a line (*bottom*) and a half plane (*top*)

We refer to $\mathcal{Q}^{(1)}$ and $\mathcal{Q}^{(2)}$ as the two *sectors* of $\mathcal{Q}$. Wave functions are complex-valued functions on $\mathcal{Q}$; any such function can be specified by specifying $\psi^{(1)}$ and $\psi^{(2)}$, the restrictions of ψ to $\mathcal{Q}^{(1)}$ and $\mathcal{Q}^{(2)}$ (called the sectors of ψ). To obtain a Hilbert space $\mathscr{H}$, we regard $\mathcal{Q}$ as a measure space with measure μ defined in the obvious way by

$$\mu(S) = \lambda^{(1)}\big(S \cap \mathcal{Q}^{(1)}\big) + \lambda^{(2)}\big(S \cap \mathcal{Q}^{(2)}\big) \tag{1}$$

for measurable sets $S \subseteq \mathcal{Q}$ with $\lambda^{(n)}$ the Lebesgue measure (n-dimensional volume) in $\mathbb{R}^n$, and take $\mathscr{H} = L^2(\mathcal{Q}, \mu)$. That is, the inner product is given by

$$\langle \psi | \phi \rangle = \int\limits_{\mathcal{Q}^{(1)}} dx\, \psi^{(1)}(x)^*\, \phi^{(1)}(x) + \int\limits_{\mathcal{Q}^{(2)}} dx\, dy\, \psi^{(2)}(x,y)^*\, \phi^{(2)}(x,y)\,. \tag{2}$$

Equivalently,

$$\mathscr{H} = \mathscr{H}^{(1)} \oplus \mathscr{H}^{(2)} \tag{3}$$

with

$$\mathscr{H}^{(n)} = L^2\big(\mathcal{Q}^{(n)}, \lambda^{(n)}\big)\,. \tag{4}$$

The configuration space $\mathcal{Q}$ has a *boundary*

$$\partial\mathcal{Q} = \big\{(x,y) \in \mathbb{R}^2 : y = 0\big\}\,. \tag{5}$$

That is, $\mathcal{Q}^{(2)}$ has a boundary, while the boundary of $\mathcal{Q}^{(1)}$ is empty. We call any non-boundary point an *interior point*.

2.2 Interior–Boundary Condition and Hamiltonian

We now impose a boundary condition on ψ. Usual boundary conditions are conditions on the value or a derivative of ψ at a boundary point. However, our boundary condition, which we call an *interior–boundary condition* (IBC), relates the value (or a derivative) of ψ at a boundary point to the value of ψ at an interior point; in this case, the boundary point $(x,0) \in \partial\mathcal{Q}^{(2)}$ gets compared to the point $x \in \mathcal{Q}^{(1)}$, which is an interior point in a different sector. The IBC reads:

$$\psi^{(2)}(x,0) = -\tfrac{2mg}{\hbar^2}\, \psi^{(1)}(x) \tag{6}$$

for every $x \in \mathbb{R}$. Here, $m > 0$ is a mass parameter and $g > 0$ a coupling constant. Note that the IBC is a linear condition. We elucidate below how one can

arrive at considering this condition. The IBC (6) goes together with the following Hamiltonian H:

$$(H\psi)^{(1)}(x) = -\tfrac{\hbar^2}{2m}\partial_x^2\psi^{(1)}(x) + g\,\partial_y\psi^{(2)}(x,0) \tag{7a}$$

$$(H\psi)^{(2)}(x,y) = -\tfrac{\hbar^2}{2m}\Big(\partial_x^2 + \partial_y^2\Big)\psi^{(2)}(x,y) \quad \text{for } y > 0\,. \tag{7b}$$

It consists of the free Schrödinger operators and a further term that links $\psi^{(1)}$ to $\psi^{(2)}$. Note that H acts linearly on $\psi = (\psi^{(1)}, \psi^{(2)})$. In order to understand the effect of the additional term, and why (7) can be expected to define a unitary time evolution, we need to consider the balance equation for the probability current.

2.3 Probability Current and Probability Balance

The well-known probability current vector field associated with the free Schrödinger Hamiltonian $-(\hbar^2/2m)\nabla^2$ on $\mathbb{R}^n$ has the form

$$j = \tfrac{\hbar}{m}\,\mathrm{Im}\big[\psi^*\nabla\psi\big] \tag{8}$$

and satisfies a continuity equation with the probability density $\rho = |\psi|^2$,

$$\partial_t\rho = -\nabla\cdot j\,. \tag{9}$$

Generally, it follows from the Schrödinger equation $i\hbar\partial_t\psi = H\psi$ that

$$\frac{\partial|\psi(q)|^2}{\partial t} = \tfrac{2}{\hbar}\,\mathrm{Im}\Big[\psi(q)^*(H\psi)(q)\Big] \tag{10}$$

at any configuration q, and for $H = -(\hbar^2/2m)\nabla^2$ the right-hand side becomes that of (9).

When considering a configuration space with boundary as in our example, the possibility arises of a probability current into the boundary, which can mean a loss of overall probability and thus a breakdown of unitarity. This can be avoided by boundary conditions such as a Dirichlet condition

$$\psi^{(2)}(x,0) = 0 \tag{11}$$

or a Neumann condition

$$\partial_y\psi^{(2)}(x,0) = 0\,. \tag{12}$$

Either of these conditions forces the current j to have vanishing normal component at every boundary point, leading to zero current into the boundary. The IBC setup, in contrast, allows nonvanishing current into the boundary while compensating this loss by a gain in probability on a different sector. In fact, the balance equation for the probability density in the first sector reads

$$\frac{\partial|\psi^{(1)}|^2}{\partial t} = \tfrac{2}{\hbar}\,\mathrm{Im}\Big[\psi^{(1)}(x)^*(H\psi)^{(1)}(x)\Big] \tag{13a}$$

$$= -\partial_x j^{(1)}(x) + \tfrac{2}{\hbar}\,\mathrm{Im}\Big[\psi^{(1)}(x)^*\, g\,\partial_y\psi^{(2)}(x,0)\Big] \tag{13b}$$

$$= -\partial_x j^{(1)}(x) - \tfrac{2g}{\hbar}\,\mathrm{Im}\Big[\tfrac{\hbar^2}{2mg}\psi^{(2)}(x,0)^*\,\partial_y\psi^{(2)}(x,0)\Big] \tag{13c}$$

$$= -\partial_x j^{(1)}(x) - \tfrac{\hbar}{m}\,\mathrm{Im}\Big[\psi^{(2)}(x,0)^*\,\partial_y\psi^{(2)}(x,0)\Big] \tag{13d}$$

$$= -\partial_x j^{(1)}(x) - j_y^{(2)}(x,0)\,, \tag{13e}$$

where we have used first (10) in (13a), then (7a) in (13b), then (6) in (13c), and then (8) in (13e), writing $j_y^{(2)}$ for the y-component of the 2-vector $j^{(2)}$. The last Eq. (13e) means that on $\mathcal{Q}^{(1)}$, $|\psi|^2$ changes due to two factors: transport along $\mathcal{Q}^{(1)}$ as governed by $j^{(1)}$, plus a second term signifying gain or loss in probability that compensates exactly the loss or gain in $\mathcal{Q}^{(2)}$ due to current into the boundary, since the usual continuity Eq. (9) holds in the interior of $\mathcal{Q}^{(2)}$. In this way, the overall probability $p^{(1)}(t) + p^{(2)}(t)$, with

$$p^{(1)}(t) := \int_{\mathcal{Q}^{(1)}} dx\,\big|\psi^{(1)}(x,t)\big|^2\,, \quad p^{(2)}(t) := \int_{\mathcal{Q}^{(2)}} dx\,dy\,\big|\psi^{(2)}(x,y,t)\big|^2\,, \tag{14}$$

is conserved, while probability may well be exchanged between $\mathcal{Q}^{(1)}$ and $\mathcal{Q}^{(2)}$, so that $p^{(1)}(t)$ and $p^{(2)}(t)$ are not individually conserved.

Readers may find it useful to visualize the probability flow in terms of Bohmian trajectories [7]. The Bohmian configuration corresponds to a random point Q_t in configuration space that moves in a way designed to ensure that Q_t has probability distribution $|\psi(t)|^2$ for every t. In our example, this distribution entails, when $\psi^{(1)}$ and $\psi^{(2)}$ are both non-zero, that Q_t lies in $\mathcal{Q}^{(1)}$ with probability $p^{(1)}(t)$ and in $\mathcal{Q}^{(2)}$ with probability $p^{(2)}(t)$. If in $\mathcal{Q}^{(2)}$, Q_t moves according to Bohm's law of motion

$$\frac{dQ_t}{dt} = \frac{j^{(2)}(Q_t,t)}{\rho^{(2)}(Q_t,t)} \tag{15}$$

until Q_t hits the boundary at $(X, 0)$, at which moment the configuration jumps[1] to $X \in \mathcal{Q}^{(1)}$. Once in $\mathcal{Q}^{(1)}$, the configuration moves according to Bohm's law of motion, i.e.,

$$\frac{dQ_t}{dt} = \frac{j^{(1)}(Q_t, t)}{\rho^{(1)}(Q_t, t)}\,, \tag{16}$$

and during any time interval of infinitesimal length dt, $Q_t = X_t$ has probability

$$\sigma(X_t, t)\, dt = \frac{\max\{0, j^{(2)}(X_t, 0, t)\}}{\rho^{(1)}(X_t, t)}\, dt\,, \tag{17}$$

to jump to the point $(X_t, 0)$ on the boundary of $\mathcal{Q}^{(2)}$ and continue from there into the interior of $\mathcal{Q}^{(2)}$ according to (15). From these laws it follows that if Q_t is $|\psi(t)|^2$ distributed for $t = 0$, then Q_t is $|\psi(t)|^2$ distributed also for $t > 0$ [7].

On another matter, it may seem from the defining Eqs. (7) of H that H cannot be Hermitian because there is no Hermitian conjugate to the term $g\,\partial_y \psi^{(2)}(x, 0)$ in (7a). However, the conservation of probability just discussed implies that there is no need for such a term; rather, the IBC replaces it.

Let us return once more to the calculation (13) to understand how one arrives at the Hamiltonian (7) and the IBC (6). Suppose we want (13e) to hold, i.e., we want an additional term in the balance equation for $\rho^{(1)}$ that compensates the loss or gain of probability in $\mathcal{Q}^{(2)}$ due to current into the boundary. Then we have to have, in the expression for $(H\psi)^{(1)}$, an additional term T_2 beyond $-\frac{\hbar^2}{2m}\partial_x^2 \psi^{(1)}(x)$, and in order to go from (13a) to (13d) we need that

$$\tfrac{2}{\hbar}\,\mathrm{Im}\Big[\psi^{(1)}(x)^*\, T_2\Big] = -\tfrac{\hbar}{m}\,\mathrm{Im}\Big[\psi^{(2)}(x, 0)^*\, \partial_y \psi^{(2)}(x, 0)\Big]\,. \tag{18}$$

This situation suggests that T_2 should involve $\psi^{(2)}$. Since T_2 needs to be linear in ψ, we need another ingredient that will allow us to replace the $\psi^{(1)}(x)^*$ on the left-hand side by a term involving $\psi^{(2)}$, thus leading to an IBC. One possibility is that $\psi^{(2)}(x, 0)^*$ on the right-hand side is proportional to $\psi^{(1)}(x)^*$ by virtue of the IBC, and that the term $\partial_y \psi^{(2)}(x, 0)$ comes from T_2, and that leads to the equations we gave above, with an arbitrary choice of the coupling constant g. (In fact, we may allow g to be negative or even complex if we replace g by g^* in (6). However, this does not really lead to more possibilities, as the resulting time evolution is unitarily

[1] An alternative way of looking at the situation, without jumps, arises from identifying $\mathcal{Q}^{(1)}$ with the boundary of $\mathcal{Q}^{(2)}$; this is described under the name "radical topology" of $\mathcal{Q}$ in [7]. Such an identification must be used with care, for example because the measure on $\mathcal{Q}$ is still given by (1) whereas boundaries usually have measure zero, and because the Laplacian on $\mathcal{Q}^{(1)}$ does not have a ∂_y^2 term. If we make this identification, which goes particularly naturally together with the IBC (6) if $-2mg/\hbar^2 = 1$, then the Bohmian configuration does not jump, but simply moves along the boundary $\partial\mathcal{Q}^{(2)} = \mathcal{Q}^{(1)}$ after reaching it.

equivalent to the one with real coupling constant $|g|$. That is because if ψ satisfies (6) with $g \to g^*$ and (7) then $\tilde{\psi}$ with $\tilde{\psi}^{(2)} = \frac{g}{|g|}\psi^{(2)}$, $\tilde{\psi}^{(1)} = \psi^{(1)}$ satisfies (6) and (7) with $g \to |g|$.)

2.4 Neumann vs. Dirichlet Conditions

Another possibility for fulfilling (18) becomes obvious when re-writing

$$\mathrm{Im}\Big[\psi^{(2)}(x,y)^*\ \partial_y\psi^{(2)}(x,y)\Big] \quad \text{as} \quad -\mathrm{Im}\Big[\partial_y\psi^{(2)}(x,y)^*\ \psi^{(2)}(x,y)\Big], \tag{19}$$

viz., that $\partial_y\psi^{(2)}(x,0)^*$ is proportional to $\psi^{(1)}(x)^*$, thus leading to a different IBC, while T_2 is proportional to $\psi^{(2)}(x,0)$. This leads to the equations

$$\partial_y\psi^{(2)}(x,0) = +\tfrac{2mg}{\hbar^2}\psi^{(1)}(x) \qquad \text{(IBC)} \tag{20a}$$

$$(H\psi)^{(1)}(x) = -\tfrac{\hbar^2}{2m}\partial_x^2\psi^{(1)}(x) + g\,\psi^{(2)}(x,0) \tag{20b}$$

$$(H\psi)^{(2)}(x,y) = -\tfrac{\hbar^2}{2m}\Big(\partial_x^2+\partial_y^2\Big)\psi^{(2)}(x,y) \quad \text{for } y>0\,. \tag{20c}$$

instead of (6) and (7), which we repeat here for comparison:

$$\psi^{(2)}(x,0) = -\tfrac{2mg}{\hbar^2}\psi^{(1)}(x) \qquad \text{(IBC)} \tag{21a}$$

$$(H\psi)^{(1)}(x) = -\tfrac{\hbar^2}{2m}\partial_x^2\psi^{(1)}(x) + g\,\partial_y\psi^{(2)}(x,0) \tag{21b}$$

$$(H\psi)^{(2)}(x,y) = -\tfrac{\hbar^2}{2m}\Big(\partial_x^2+\partial_y^2\Big)\psi^{(2)}(x,y) \quad \text{for } y>0\,. \tag{21c}$$

That is, while the original IBC (21a) was of Dirichlet type (in that it specifies the value of $\psi^{(2)}$ on the boundary), the alternative IBC (20a) is of Neumann type (in that it specifies the normal derivative of $\psi^{(2)}$ on the boundary). This change is accompanied by a change of the term T_2 in the equation for the Hamiltonian and leads to a different time evolution.

Another type of boundary condition often considered besides the Neumann condition

$$\frac{\partial\psi}{\partial n}\Big|_{\partial\mathcal{Q}} = 0 \tag{22}$$

and the Dirichlet condition

$$\psi\Big|_{\partial\mathcal{Q}} = 0 \tag{23}$$

is the Robin boundary condition

$$\alpha\psi + \beta \frac{\partial \psi}{\partial n}\Big|_{\partial \mathcal{Q}} = 0 \tag{24}$$

with constants $\alpha, \beta \in \mathbb{R}$. Correspondingly, another possibility for the IBC and the equations for H is

$$\big(\alpha + \beta\partial_y\big)\psi^{(2)}(x,0) = \tfrac{2mg}{\hbar^2}\psi^{(1)}(x) \qquad \text{(IBC)} \tag{25a}$$

$$(H\psi)^{(1)}(x) = -\tfrac{\hbar^2}{2m}\partial_x^2\psi^{(1)}(x) + g\left(\gamma + \delta\partial_y\right)\psi^{(2)}(x,0) \tag{25b}$$

$$(H\psi)^{(2)}(x,y) = -\tfrac{\hbar^2}{2m}\Big(\partial_x^2 + \partial_y^2\Big)\psi^{(2)}(x,y) \quad \text{for } y > 0 \tag{25c}$$

with constants $\alpha, \beta, \gamma, \delta \in \mathbb{R}$ such that $\alpha\delta - \beta\gamma = -1$.

2.5 Rigorous, Self-Adjoint Hamiltonian

Readers that are mathematicians may be interested in the rigorous definition of the Hamiltonian, which we give here for the Dirichlet-type condition (6). The domain $\mathscr{D}$ consists of functions in $\mathscr{H}$ that satisfy the IBC. More precisely, let

$$\mathscr{D}_0 = H^2(\mathbb{R}) \oplus H^2\big(\mathbb{R} \times [0,\infty)\big) \subseteq \mathscr{H}^{(1)} \oplus \mathscr{H}^{(2)}\,, \tag{26}$$

where H^2 denotes the second Sobolev space, and $H^2\big(\mathbb{R} \times [0,\infty)\big)$ contains the restriction of functions in $H^2(\mathbb{R}^2)$ to $\mathbb{R} \times [0,\infty)$. By the Sobolev embedding theorem (e.g., [1, p. 85]), any element $\psi^{(2)}$ of $H^2(\mathbb{R}^2)$ possesses a unique restriction $f \in L^2(\mathbb{R})$ to the subspace $\mathbb{R} \times \{0\}$. The IBC (6), understood as the condition $f = (-2mg/\hbar^2)\psi^{(1)}$, is thus meaningful for every $\psi \in \mathscr{D}_0$, and we can define

$$\mathscr{D} = \left\{\psi \in \mathscr{D}_0 : f = -\tfrac{2mg}{\hbar^2}\,\psi^{(1)}\right\}. \tag{27}$$

Likewise, the y-derivative of any element of $H^2(\mathbb{R}^2)$ lies in $H^1(\mathbb{R}^2)$ and possesses, by the Sobolev embedding theorem, a unique restriction $h \in L^2(\mathbb{R})$ to the subspace $\mathbb{R} \times \{0\}$. Thus, the Hamiltonian can be defined on $\mathscr{D}$ by

$$(H\psi)^{(1)}(x) = -\tfrac{\hbar^2}{2m}\partial_x^2\psi^{(1)}(x) + g\,h(x) \tag{28a}$$

$$(H\psi)^{(2)}(x,y) = -\tfrac{\hbar^2}{2m}\Big(\partial_x^2 + \partial_y^2\Big)\psi^{(2)}(x,y)\,, \tag{28b}$$

and one can show:

Theorem 1 *$\mathscr{D}$ is dense in $\mathscr{H}$, and H is self-adjoint on the domain $\mathscr{D}$.*

3 Particle Creation via IBC

We now transfer the IBC approach to a simple model of particle creation and annihilation.

3.1 Configuration Space and Hilbert Space

Suppose that x-particles can emit and absorb y-particles, and consider a single x-particle fixed at the origin. For simplicity, we take the x- and y-particles to be spinless, and we intend to cut off from the Fock space for the y-particles any sector with particle number 2 or higher. To this end, we consider only y-configurations with 0 or 1 particle, so $\mathcal{Q} = \mathcal{Q}^{(0)} \cup \mathcal{Q}^{(1)}$, where $\mathcal{Q}^{(0)}$ has a single element (the empty configuration $\emptyset$), while $\mathcal{Q}^{(1)}$ is a copy of physical space $\mathbb{R}^3$. Wave functions are again functions $\psi : \mathcal{Q} \to \mathbb{C}$, and the Hilbert space is

$$\mathscr{H} = \mathscr{H}^{(0)} \oplus \mathscr{H}^{(1)} = \mathbb{C} \oplus L^2(\mathbb{R}^3)\,, \tag{29}$$

which has inner product

$$\langle \psi | \phi \rangle = \psi^{(0)*} \phi^{(0)} + \int_{\mathcal{Q}^{(1)}} d^3\boldsymbol{y}\; \psi^{(1)}(\boldsymbol{y})^*\, \phi^{(1)}(\boldsymbol{y})\,. \tag{30}$$

Writing $\boldsymbol{y} \in \mathcal{Q}^{(1)}$, the position of the y-particle, in spherical coordinates $(r, \boldsymbol{\omega})$ with $0 \le r < \infty$ and $\boldsymbol{\omega} \in \mathbb{S}^2$ (the unit sphere in $\mathbb{R}^3$), we can think of $\mathcal{Q}^{(1)}$ as

$$\mathcal{Q}^{(1)} = [0, \infty) \times \mathbb{S}^2 \tag{31}$$

with Riemannian metric

$$ds^2 = dr^2 + r^2\, d\boldsymbol{\omega}^2 \tag{32}$$

(with $d\boldsymbol{\omega}^2$ the 2-dimensional metric on the sphere). The inner product then reads

$$\langle \psi | \phi \rangle = \psi^{(0)*} \phi^{(0)} + \int_0^\infty dr \int_{\mathbb{S}^2} d^2\boldsymbol{\omega}\; r^2\, \psi^{(1)}(r, \boldsymbol{\omega})^*\, \phi^{(1)}(r, \boldsymbol{\omega})\,, \tag{33}$$

and the Laplace operator becomes

$$\Delta = \partial_r^2 + \tfrac{2}{r}\partial_r + \tfrac{1}{r^2}\Delta_{\boldsymbol{\omega}} \tag{34}$$

with $\Delta_{\boldsymbol{\omega}}$ the Laplace operator on the sphere.

3.2 IBC and Hamiltonian

The relevant boundary of $\mathcal{Q}^{(1)}$ is the set $\partial\mathcal{Q}^{(1)} = \{r = 0\}$, which corresponds to the origin (the location of the x-particle) in $\mathbb{R}^3$ and is represented by the surface $\{0\}\times\mathbb{S}^2$ in spherical coordinates. Probability current into this boundary corresponds to the annihilation of the y-particle and current out of the boundary to the creation of a y-particle. (In terms of Bohmian trajectories, when a trajectory Q_t in $\mathcal{Q}^{(1)}$ hits $\{r = 0\}$, so that the y-particle reaches the origin, then Q_t jumps to $\emptyset \in \mathcal{Q}^{(0)}$, so that the y-particles gets absorbed by the x-particle; conversely, if $Q_t = \emptyset$, then at a random time, governed by a law similar to (17), Q_t jumps to $\{r = 0\}$ and moves into the interior, $\{r > 0\}$, so that a y-particle gets emitted by the x-particle.)

In this setup, the IBC analogous to (6) reads: For every $\boldsymbol{\omega} \in \mathbb{S}^2$,

$$\lim_{r\searrow 0}\big(r\psi^{(1)}(r\boldsymbol{\omega})\big) = -\tfrac{mg}{2\pi\hbar^2}\,\psi^{(0)}\,. \tag{35}$$

The Hamiltonian analogous to (7) is

$$(H\psi)^{(0)} = \tfrac{g}{4\pi}\int_{\mathbb{S}^2} d^2\boldsymbol{\omega}\,\lim_{r\searrow 0}\partial_r\Big(r\psi^{(1)}(r\boldsymbol{\omega})\Big) \tag{36a}$$

$$(H\psi)^{(1)}(r\boldsymbol{\omega}) = -\tfrac{\hbar^2}{2m}\Big(\partial_r^2 + \tfrac{2}{r}\partial_r + \tfrac{1}{r^2}\Delta_{\boldsymbol{\omega}}\Big)\psi^{(1)}(r\boldsymbol{\omega}) \quad \text{for } r > 0\,. \tag{36b}$$

It can be shown [10] that (36) defines a self-adjoint operator H on a dense domain $\mathscr{D}$ in $\mathscr{H}$ consisting of functions satisfying the IBC (35). (It turns out that elements of $\mathscr{D}$ satisfy a stronger version of (35) that has the limit $r \to 0$ replaced by the limit $r\boldsymbol{\omega} \to \mathbf{0}$; that is, the stronger version does not demand that the limit be taken *in the radial direction, keeping* $\boldsymbol{\omega}$ *constant*, but allows any way of approaching the boundary surface, even without a limiting value for $\boldsymbol{\omega}$.)

3.3 Remarks

1. $1/r$ *asymptotics.* As a consequence of the IBC (35), whenever $\psi^{(0)}$ is nonzero then $\psi^{(1)}$ diverges at $\{r = 0\}$ like $1/r$. This behavior is to be expected, for a reason that is perhaps most easily appreciated by means of the following simple approximation: Consider an ensemble of systems in which the y-particle moves at unit speed towards the origin and gets annihilated when it reaches the origin; that is, the motion follows the equation of motion

$$\frac{d\boldsymbol{y}}{dt} = -\frac{\boldsymbol{y}}{|\boldsymbol{y}|}\,. \tag{37}$$

Suppose first that the ensemble density is uniform over a spherical shell of radius r and thickness dr; as the members of the ensemble move inwards, the density increases like $1/r^2$ since the area of a sphere is proportional to r^2 and the thickness dr remains constant. As a consequence, the stationary density for the particle motion (37) diverges at the origin like $1/r^2$. It thus comes as no surprise that $|\psi|^2$ on $\mathcal{Q}^{(1)}$ should diverge at the origin like $1/r^2$, and so $|\psi|$ should diverge like $1/r$. Conversely, the $1/r$ divergence of $\psi^{(1)}$ at the boundary $\{r = 0\}$ makes the r factor in the IBC (35) necessary, as $\lim_{r\searrow 0} \psi^{(1)}(r\boldsymbol{\omega})$ (without the r factor) does not exist.

2. H_{IBC} *is not a perturbation of* H_{free}. We note that H_{IBC} cannot be decomposed into a sum of two self-adjoint operators $H_{\text{free}} + H_{\text{interaction}}$. As a consequence, H_{IBC} cannot be found when studying Hamiltonians of the form $H_{\text{free}} + H_{\text{interaction}}$. That is because the domain $\mathscr{D}_{IBC}$ of H_{IBC} is different from the free domain $\mathscr{D}_{\text{free}}$; specifically, functions in $\mathscr{D}_{IBC}$ diverge like $1/r$ at $\{r = 0\}$, while functions in the free domain (the second Sobolev space) stay bounded at $\{r = 0\}$ and thus yield $\lim_{r\searrow 0}\big(r\psi^{(1)}(r\boldsymbol{\omega})\big) = 0$. The Laplacian is not self-adjoint on $\mathscr{D}_{IBC}$ (i.e., does not conserve probability) because it allows a nonzero flux of probability into the boundary $\{r = 0\}$, while the additional term in H_{IBC} compensates that flux by adding it to $\mathcal{Q}^{(0)}$.
3. *Comparison to a known boundary condition.* Boundary conditions at $\{r = 0\}$ have been used before; in particular, Bethe and Peierls [3] introduced the boundary condition

$$\lim_{r\searrow 0}\Big[\partial_r\big(r\psi(r\boldsymbol{\omega})\big) + \alpha r\psi(r\boldsymbol{\omega})\Big] = 0 \quad \forall \boldsymbol{\omega} \in \mathbb{S}^2 \tag{38}$$

with given constant $\alpha \in \mathbb{R}$ and wave function $\psi : \mathbb{R}^3 \to \mathbb{C}$, for the purpose of making precise what it means to have on $\mathscr{H} = L^2(\mathbb{R}^3, \mathbb{C})$ a Schrödinger equation with a Dirac δ function as the potential,

$$H = -\frac{\hbar^2}{2m}\nabla^2 + g\,\delta^3(\boldsymbol{x})\,, \tag{39}$$

see [2] for more detail. Note that (38) leads to zero current into $\{r = 0\}$, as that current is

$$J_0 = -\lim_{r\searrow 0}\int_{\mathbb{S}^2} d^2\boldsymbol{\omega}\; r^2\, j_r(r\boldsymbol{\omega}) \tag{40a}$$

$$= -\lim_{r\searrow 0}\int_{\mathbb{S}^2} d^2\boldsymbol{\omega}\; r^2\, \tfrac{\hbar}{m}\,\mathrm{Im}\big[\psi(r\boldsymbol{\omega})^*\,\partial_r\psi(r\boldsymbol{\omega})\big] \tag{40b}$$

$$= -\lim_{r\searrow 0}\int_{\mathbb{S}^2} d^2\boldsymbol{\omega}\; r\, \tfrac{\hbar}{m}\,\mathrm{Im}\big[\psi(r\boldsymbol{\omega})^*\,\partial_r\big(r\psi(r\boldsymbol{\omega})\big)\big] \tag{40c}$$

$$\overset{(38)}{=} \lim_{r \searrow 0} \int_{\mathbb{S}^2} d^2\boldsymbol{\omega}\; r\, \tfrac{\hbar}{m} \operatorname{Im}\big[\psi(r\boldsymbol{\omega})^*\, \alpha r \psi(r\boldsymbol{\omega})\big] \tag{40d}$$

$$= 0\,. \tag{40e}$$

In contrast, the IBC (35), which we may re-write in the form

$$\lim_{r \searrow 0} r\psi(r\boldsymbol{\omega}) = \alpha\, \psi(\emptyset) \quad \forall \boldsymbol{\omega} \in \mathbb{S}^2 \tag{41}$$

with suitable constant $\alpha \in \mathbb{R}$, leads to nonzero current into $\{r = 0\}$. Moreover, the IBC (41) involves two sectors of ψ, while the Bethe–Peierls boundary condition (38) involves only one.

4 IBC in QFT

The application of interior–boundary conditions in quantum field theory is based on the particle-position representation, in which a QFT becomes a kind of quantum mechanics with particle creation and annihilation.

In relativistic QFT, there are issues with the particle-position representation, but they do not seem fatal for the IBC approach: (i) Some QFTs appear to lead to an infinite number of particles (e.g., [5]); a configuration space for an infinite number of particles will be more difficult, but not impossible, to deal with. (ii) Photons are believed not to have a good position representation (e.g., [4]). However, photon wave functions are believed to be mathematically equivalent to (complexified) classical Maxwell fields [4], and that may be good enough for IBCs. (iii) The construction of the configuration space is based on a choice of hypersurface in space-time $\mathscr{M}$; however, the use of multi-time wave functions [16] would avoid such a choice, as such wave functions are defined on (the spacelike subset of) $\cup_{n=0}^{\infty} \mathscr{M}^n$.

We focus here on non-relativistic models, for which the relevant Hilbert spaces are bosonic or fermionic Fock spaces $\mathscr{F}^{\pm}$, or tensor products of such spaces. The corresponding configuration space contains configurations of any number of particles (see Fig. 2),

$$\mathcal{Q} = \bigcup_{n=0}^{\infty} \mathcal{Q}^{(n)} = \bigcup_{n=0}^{\infty} (\mathbb{R}^3)^n\,. \tag{42}$$

In fact, for spinless particles, $\mathscr{F}^{\pm}$ consists of those functions $\psi : \mathcal{Q} \to \mathbb{C}$ that are (anti-)symmetric on every sector $\mathcal{Q}^{(n)}$ and that are square-integrable in the sense

$$\sum_{n=0}^{\infty} \int_{\mathbb{R}^{3n}} d^{3n}q\, |\psi(q)|^2 < \infty\,. \tag{43}$$

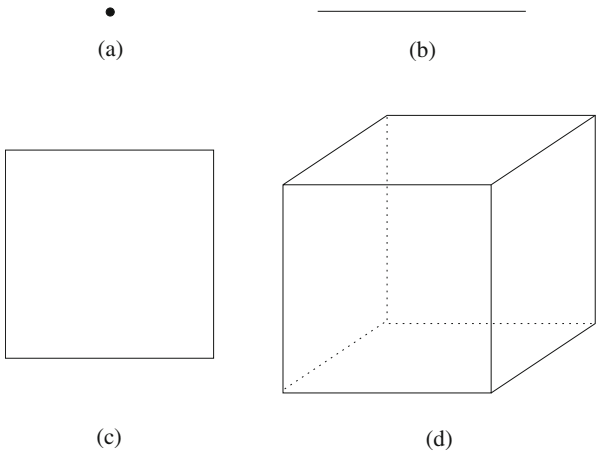


Fig. 2 The configuration space considered in (42) is the disjoint union of n-particle configuration spaces (shown here for 1 rather than 3 space dimensions); parts (**a**) through (**d**) show the 0-particle through 3-particle sector of the configuration space $\mathcal{Q}$

It is sometimes preferable to consider a slightly different configuration space and remove the collision configurations (i.e., those with two or more particles at the same location),

$$\mathcal{Q}^{(n)} = \left\{(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n) \in (\mathbb{R}^3)^n : \boldsymbol{x}_i \neq \boldsymbol{x}_j \text{ for } i \neq j\right\}. \tag{44}$$

Alternatively, it is sometimes desirable to consider *unordered* configurations (e.g., [8]),

$$\mathcal{Q}^{(n)} = \left\{q \subset \mathbb{R}^3 : \#q = n\right\}. \tag{45}$$

4.1 Model QFT

Suppose again that x-particles can emit and absorb y-particles. In [11] we study a model QFT adapted from [17, p. 339], [15], and the Lee model [14], starting out from the following, UV divergent expression for the Hamiltonian:

$$\begin{aligned} H_{\text{orig}} = {} & \tfrac{\hbar^2}{2m_x} \int d^3\boldsymbol{q}\, \nabla a_x^\dagger(\boldsymbol{q})\, \nabla a_x(\boldsymbol{q}) \\ & + \tfrac{\hbar^2}{2m_y} \int d^3\boldsymbol{q}\, \nabla a_y^\dagger(\boldsymbol{q})\, \nabla a_y(\boldsymbol{q}) + E_0 \int d^3\boldsymbol{q}\, a_y^\dagger(\boldsymbol{q})\, a_y(\boldsymbol{q}) \\ & + g \int d^3\boldsymbol{q}\, a_x^\dagger(\boldsymbol{q}) \left(a_y(\boldsymbol{q}) + a_y^\dagger(\boldsymbol{q})\right) a_x(\boldsymbol{q}). \end{aligned} \tag{46}$$

Here, † denotes the adjoint operator, and $a(\boldsymbol{q})$ and $a^\dagger(\boldsymbol{q})$ are the annihilation and creation operators for either an x- or a y-particle at location $\boldsymbol{q}$ in position space; $g > 0$ a coupling constant, and $E_0 \geq 0$ the amount of energy required to create a y-particle. The Hilbert space is

$$\mathscr{H} = \mathscr{F}_x^- \otimes \mathscr{F}_y^+ , \tag{47}$$

and the configuration space is

$$\mathcal{Q} = \bigcup_{m,n=0}^{\infty} (\mathbb{R}^3_x)^m \times (\mathbb{R}^3_y)^n . \tag{48}$$

We consider here a simplified version of this model, in which we allow only a single x-particle (but any number of y-particles), and this x-particle cannot move but is fixed at the origin $\mathbf{0} \in \mathbb{R}^3$; such models are sometimes connected with the name of van Hove [6, 21]. The Hilbert space of this model is $\mathscr{H} = \mathscr{F}_y^+$, and its configuration space is $\mathcal{Q} = \mathcal{Q}_y = \bigcup_{n=0}^{\infty} (\mathbb{R}^3_y)^n$. For a point $y = (\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n)$ in configuration space $\mathcal{Q}$, we will often use the notation y^n to convey that this configuration has n y-particles. The original Hamiltonian (46) simplifies in this model to

$$\begin{aligned} H_{\text{orig}} = {} & \tfrac{\hbar^2}{2m_y} \int d^3\boldsymbol{q}\, \nabla a_y^\dagger(\boldsymbol{q})\, \nabla a_y(\boldsymbol{q}) + E_0 \int d^3\boldsymbol{q}\, a_y^\dagger(\boldsymbol{q})\, a_y(\boldsymbol{q}) \\ & + g\left(a_y(\mathbf{0}) + a_y^\dagger(\mathbf{0})\right) . \end{aligned} \tag{49}$$

In the particle-position representation, in which elements ψ of $\mathscr{H}$ are regarded as functions $\psi : \mathcal{Q} \to \mathbb{C}$, this reads

$$\begin{aligned} (H_{\text{orig}}\psi)(y^n) = {} & -\tfrac{\hbar^2}{2m_y} \sum_{j=1}^{n} \nabla_{\boldsymbol{y}_j}^2 \psi(y^n) + nE_0 \psi(y^n) \\ & + g\sqrt{n+1}\, \psi\left(y^n, \mathbf{0}\right) \\ & + \frac{g}{\sqrt{n}} \sum_{j=1}^{n} \delta^3(\boldsymbol{y}_j)\, \psi\left(y^n \setminus \boldsymbol{y}_j\right) , \end{aligned} \tag{50}$$

with the notation $y^n \setminus \boldsymbol{y}_j$ meaning $(\boldsymbol{y}_1, \ldots, \boldsymbol{y}_{j-1}, \boldsymbol{y}_{j+1}, \ldots, \boldsymbol{y}_n)$ (leaving out $\boldsymbol{y}_j$). H_{orig} is UV divergent because the wave function of the newly created y-particle, $\delta^3(\boldsymbol{y})$, does not lie in $L^2(\mathbb{R}^3)$ (or, has infinite energy).

To obtain a well-defined Hamiltonian, a standard approach is to "smear out" the x-particle at $\mathbf{0}$ with "charge distribution" $\varphi(\cdot)$, where the "cut-off function" φ lies in $L^2(\mathbb{R}^3, \mathbb{C})$:

$$\begin{aligned}(H_{\text{cutoff}}\psi)(y^n) = &-\tfrac{\hbar^2}{2m_y}\sum_{j=1}^{n}\nabla_{y_j}^2\psi(y^n) + nE_0\psi(y^n)\\ &+ g\sqrt{n+1}\int_{\mathbb{R}^3} d^3\mathbf{y}\,\varphi(\mathbf{y})^*\,\psi\big(y^n,\mathbf{y}\big)\\ &+ \frac{g}{\sqrt{n}}\sum_{j=1}^{n}\varphi(\mathbf{y}_j)\,\psi\big(y^n\setminus\mathbf{y}_j\big)\,.\end{aligned} \tag{51}$$

4.2 IBC Approach

What the IBC approach yields for this model is just the extension of the equations of Sect. 3 to an unbounded number of y-particles. The relevant boundary of $\mathcal{Q}$ consists of those configurations y^n for which a y-particle collides with the x-particle, i.e., $\mathbf{y}_j = \mathbf{0}$ for some $j \le n$; the related interior configuration is obtained by removing $\mathbf{y}_j$ (and all other y-particles at $\mathbf{0}$, if any). The Dirichlet-type IBC reads as follows: For every $y^n \in (\mathbb{R}^3 \setminus \{\mathbf{0}\})^n$ and every $j \le n$,

$$\lim_{\mathbf{y}_j\to\mathbf{0}} |\mathbf{y}_j|\,\psi(y^n) = -\tfrac{mg}{2\pi\hbar^2\sqrt{n}}\,\psi(y^n\setminus\mathbf{y}_j) \tag{52}$$

with $m = m_y$. The corresponding Hamiltonian is

$$\begin{aligned}(H_{IBC}\psi)(y^n) = &-\tfrac{\hbar^2}{2m}\sum_{j=1}^{n}\nabla_{y_j}^2\psi + nE_0\psi\\ &+ \frac{g\sqrt{n+1}}{4\pi}\int_{\mathbb{S}^2} d^2\boldsymbol{\omega}\,\lim_{r\searrow 0}\partial_r\Big[r\psi\big(y^n, r\boldsymbol{\omega}\big)\Big]\\ &+ \frac{g}{\sqrt{n}}\sum_{j=1}^{n}\delta^3(\mathbf{y}_j)\,\psi\big(y^n\setminus\mathbf{y}_j\big)\,.\end{aligned} \tag{53}$$

Theorem 2 ([10]) *On a certain dense subspace $\mathscr{D}_{IBC}$ of $\mathscr{H}$, the elements of which satisfy the IBC (52), the operator H_{IBC} given by (53) is well-defined and self-adjoint.*

It may seem that H_{IBC} as in (53) should have the same UV problem as H_{orig} in (50); after all, we said that the problem with H_{orig} is caused by the Dirac δ function, and the last line of (53) coincides with that of (50), and in particular

contains the same δ function. And yet, H_{IBC} is well defined and H_{orig} is not! Here is why. As in the model of Sect. 3 (see Remark 1), ψ grows like $1/r = 1/|\boldsymbol{y}_j|$ as $\boldsymbol{y}_j \to \boldsymbol{0}$ due to the IBC (52), and as readers may recall from classical electrostatics, where $1/r$ comes up as the Coulomb potential, the Laplacian of $1/r$ (which equals the charge density, according to the Poisson equation of electrostatics) is $-4\pi\delta^3(\boldsymbol{x})$. As a consequence, the Laplacian in the first row of (53) contributes a δ function, which then gets exactly canceled by the δ function in the last row of (53). That is how $H_{IBC}\psi$ can manage to be a square-integrable function on $\mathcal{Q}$.

The fact that the last line of (53) coincides with that of (50), that is, that both equations have the same term for particle creation, underlines the parallel between H_{IBC} and H_{orig} and suggests that H_{IBC} may be regarded as a precise interpretation of the formal expression (50) for H_{orig}.

At this point, readers may wonder why the formula (36b) for the Hamiltonian in the simpler creation model did not contain a δ function. The reason is merely a matter of notation, as (36) can be equivalently rewritten as

$$(H\psi)^{(0)} = \tfrac{g}{4\pi} \int_{\mathbb{S}^2} d^2\boldsymbol{\omega} \lim_{r\searrow 0} \partial_r \Big(r\psi^{(1)}(r\boldsymbol{\omega}) \Big) \tag{54a}$$

$$(H\psi)^{(1)}(\boldsymbol{y}) = -\tfrac{\hbar^2}{2m} \nabla_{\boldsymbol{y}}^2 \psi^{(1)}(\boldsymbol{y}) + g\, \delta^3(\boldsymbol{y})\, \psi^{(0)} \,. \tag{54b}$$

In (36b), we explicitly assumed $r > 0$, thus stating the action of H only *away from the origin*, so that the term involving $\delta^3(\boldsymbol{y})$ does not show up. In (53) and (54b), in contrast, we did not exclude the origin because we wanted to make the δ behavior explicit.

4.3 Remarks

4. *Positive Hamiltonian.* For $E_0 > 0$, it can be shown [10] that H_{IBC} as in (53) is a *positive* operator.
5. *Ground state.* It can be shown further [10] for $E_0 > 0$ that H_{IBC} possesses a non-degenerate ground state $\psi_{\min}$, which is

$$\psi_{\min}(\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n) = \mathcal{N} \frac{(-gm)^n}{(2\pi\hbar^2)^n \sqrt{n!}} \prod_{j=1}^{n} \frac{e^{-\sqrt{2mE_0}|\boldsymbol{y}_j|/\hbar}}{|\boldsymbol{y}_j|} \tag{55}$$

with normalization constant $\mathcal{N}$ and eigenvalue

$$E_{\min} = \frac{g^2 m \sqrt{2mE_0}}{2\pi\hbar^3} \,. \tag{56}$$

That is, the x-particle is dressed with a cloud of y-particles.

6. *Effective Yukawa potential between x-particles.* To compute the effective interaction between x-particles by exchange of y-particles, consider two x-particles fixed at $\boldsymbol{x}_1 = (0,0,0)$ and $\boldsymbol{x}_2 = (R,0,0)$; two IBCs, one at $\boldsymbol{x}_1$ and one at $\boldsymbol{x}_2$; and two creation and annihilation terms in H_{IBC}. For $E_0 > 0$, the ground state is

$$\psi_{\min}(\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n) = c_n \prod_{j=1}^{n} \sum_{i=1}^{2} \frac{e^{-\sqrt{2mE_0}|\boldsymbol{y}_j - \boldsymbol{x}_i|/\hbar}}{|\boldsymbol{y}_j - \boldsymbol{x}_i|} \tag{57}$$

with suitable factors c_n and eigenvalue

$$E_{\min} = \frac{g^2 m}{\pi\hbar^2}\left(\frac{\sqrt{2mE_0}}{\hbar} - \frac{e^{-\sqrt{2mE_0}R/\hbar}}{R}\right). \tag{58}$$

As a consequence, for any two locations $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$, the ground state energy of the y-particles, given the x-particles at $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$, is given by (58) with $R = |\boldsymbol{x}_1 - \boldsymbol{x}_2|$. Regarding this energy function of $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ as an effective potential for the x-particles (which is appropriate when the x-particles move slowly, see, e.g., [18]), we see that x-particles effectively interact through an attractive Yukawa potential, $V(R) = \text{const.} - e^{-\alpha R}/R$.

7. *Comparison to renormalization procedure.* Returning to the scenario with a single x-particle fixed at the origin, consider $H_{\text{cutoff}} = H_\varphi$ as in (51) with cutoff function φ and take the limit $\varphi \to \delta^3$. It is known [6] that, if $E_0 > 0$, there exist constants $E_\varphi \to \infty$ and a self-adjoint operator H_∞ such that

$$H_\varphi - E_\varphi \to H_\infty\,. \tag{59}$$

It can be shown [10] that

$$H_\infty = H_{IBC} + \text{const.}\,. \tag{60}$$

Note added. After completion of this article we have become aware that Equations (35) and (36) were already considered in [20] and [22].

References

1. R.A. Adams, J.J.F. Fournier, *Sobolev Spaces*, 2nd edn. (Academic, Amsterdam/Boston, 2003)
2. S. Albeverio, F. Gesztesy, R. Høegh-Krohn, H. Holden, *Solvable Models in Quantum Mechanics* (Springer, Berlin, 1988)
3. H. Bethe, R. Peierls, Quantum theory of the diplon. Proc. R. Soc. Lond. A **148**, 146–156 (1935)
4. I. Bialynicki-Birula, Photon wave function, in *Progress in Optics*, vol. XXXVI, ed. by E. Wolf (Elsevier, Amsterdam, 1996)

5. D.-A. Deckert, D. Dürr, F. Merkl, M. Schottenloher, Time-evolution of the external field problem in quantum electrodynamics. J. Math. Phys. **51**, 122301 (2010). http://arxiv.org/abs/0906.0046
6. J. Dereziński, Van Hove Hamiltonians—exactly solvable models of the infrared and ultraviolet problem. Ann. Henri Poincaré **4**, 713–738 (2003)
7. D. Dürr, S. Goldstein, S. Teufel, R. Tumulka, N. Zanghì, *Bohmian Trajectories for Hamiltonians with Interior–Boundary Conditions* (2015, in preparation)
8. S. Goldstein, J. Taylor, R. Tumulka, N. Zanghì, *Fermionic Wave Functions on Unordered Configurations* (2014, preprint). http://arxiv.org/abs/1403.3705
9. S. Keppeler, M. Sieber, *Particle Creation and Annihilation by Interior–Boundary Conditions in One Dimension* (2015, in preparation)
10. J. Lampart, J. Schmidt, S. Teufel, R. Tumulka, *Absence of Ultraviolet Divergence in Quantum Field Theories with Interior–Boundary Conditions. I. Schrödinger Operators and Fixed Sources* (2015, Preprint)
11. J. Lampart, J. Schmidt, S. Teufel, R. Tumulka, *Absence of Ultraviolet Divergence in Quantum Field Theories with Interior–Boundary Conditions. II. Schrödinger Operators and Moving Sources* (2015, in preparation)
12. J. Lampart, J. Schmidt, S. Teufel, R. Tumulka, *Absence of Ultraviolet Divergence in Quantum Field Theories with Interior–Boundary Conditions. III. Dirac Operators* (2015, in preparation)
13. L. Landau, R. Peierls, Quantenelektrodynamik im Konfigurationsraum. Z. für Phys. **62**, 188–200 (1930)
14. T.D. Lee, Some special examples in renormalizable field theory. Phys. Rev. **95**, 1329–1334 (1954)
15. E. Nelson, Interaction of nonrelativistic particles with a quantized scalar field. J. Math. Phys. **5**, 1190–1197 (1964)
16. S. Petrat, R. Tumulka, Multi-time wave functions for quantum field theory. Ann. Phys. **345**, 17–54 (2014). http://arxiv.org/abs/1309.0802
17. S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Harper and Row, New York, 1961)
18. S. Teufel, *Adiabatic Perturbation Theory in Quantum Dynamics.* Lecture Notes in Mathematics, vol. 1821 (Springer, Berlin, 2003)
19. S. Teufel, R. Tumulka, *New Type of Hamiltonians Without Ultraviolet Divergence for Quantum Field Theories* (2015, preprint). http://arxiv.org/abs/1505.04847
20. L.E. Thomas, Multiparticle Schrödinger Hamiltonians with point interactions. Phys. Rev. D **30**, 1233–1237 (1984)
21. L. van Hove, Les difficultés de divergences pour un modele particulier de champ quantifié. Physica **18**, 145–159 (1952)
22. D.R. Yafaev, On a zero-range interaction of a quantum particle with the vacuum. J. Phys. A Math. Gen. **25**, 963–978 (1992)

Causal Fermion Systems: An Overview

Felix Finster

Contents

F. Finster (✉)
Fakultät für Mathematik, Universität Regensburg, D-93040 Regensburg, Germany
e-mail: finster@ur.de

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_15

Abstract The theory of causal fermion systems is an approach to describe fundamental physics. We here introduce the mathematical framework and give an overview of the objectives and current results.

Keywords Relativistic quantum theory • Unified theories

Mathematics Subject Classification (2010). 81-02, 81-06, 81V22

Causal fermion systems were introduced in [17] as a reformulation and generalization of the setting used in the fermionic projector approach [8]. The theory of causal fermion systems is an approach to describe fundamental physics. It gives quantum mechanics, general relativity and quantum field theory as limiting cases and is therefore a candidate for a unified physical theory. In this article, we introduce the mathematical framework and give an overview of the different limiting cases. The presentation is self-contained and includes references to the corresponding research papers. The aim is not only to convey the underlying physical picture, but also to lay the mathematical foundations in a conceptually convincing way. This includes technical issues like specifying the topologies on the different spaces of functions and operators, giving a mathematical definition of an ultraviolet regularization, or specifying the maps which identify the objects of the causal fermion system with corresponding objects in Minkowski space. Also, we use a basis-independent notation whenever possible. The reader interested in a non-technical introduction is referred to [21].

1 The Abstract Framework

1.1 Basic Definitions

For conceptual clarity, we begin with the general definitions.

Definition 1.1 (causal fermion system) Given a separable complex Hilbert space $\mathcal{H}$ with scalar product $\langle .|. \rangle_{\mathcal{H}}$ and a parameter $n \in \mathbb{N}$ (the *"spin dimension"*), we let $\mathcal{F} \subset \mathrm{L}(\mathcal{H})$ be the set of all self-adjoint operators on $\mathcal{H}$ of finite rank, which (counting multiplicities) have at most n positive and at most n negative eigenvalues. On $\mathcal{F}$ we are given a positive measure ρ (defined on a σ-algebra of subsets of $\mathcal{F}$), the so-called *universal measure*. We refer to $(\mathcal{H}, \mathcal{F}, \rho)$ as a *causal fermion system*.

We remark that the separability of the Hilbert space (i.e. the assumption that $\mathcal{H}$ admits an at most countable Hilbert space basis) is not essential and could be left out. We included the separability assumption because it seems to cover all cases of physical interest and is useful if one wants to work with basis representations.

A causal fermion system describes a space-time together with all structures and objects therein (like the causal and metric structures, spinors and interacting

quantum fields). In order to single out the physically admissible causal fermion systems, one must formulate physical equations. This is accomplished with the help of an action principle which we now introduce. For any $x, y \in \mathcal{F}$, the product xy is an operator of rank at most $2n$. We denote its non-trivial eigenvalues (counting algebraic multiplicities) by $\lambda_1^{xy}, \ldots, \lambda_{2n}^{xy} \in \mathbb{C}$. We introduce the *spectral weight* $|.|$ of an operator as the sum of the absolute values of its eigenvalues. In particular, the spectral weight of the operator products xy and $(xy)^2$ is defined by

$$|xy| = \sum_{i=1}^{2n} \left|\lambda_i^{xy}\right| \qquad \text{and} \qquad \left|(xy)^2\right| = \sum_{i=1}^{2n} \left|\lambda_i^{xy}\right|^2 .$$

We introduce the Lagrangian and the action by

$$\textit{Lagrangian:} \qquad \mathcal{L}(x,y) = \left|(xy)^2\right| - \frac{1}{2n} |xy|^2 \tag{1}$$

$$\textit{action:} \qquad \mathcal{S}(\rho) = \iint_{\mathcal{F}\times\mathcal{F}} \mathcal{L}(x,y)\, d\rho(x)\, d\rho(y) . \tag{2}$$

The *causal action principle* is to minimize $\mathcal{S}$ by varying the universal measure under the following constraints:

$$\textit{volume constraint:} \qquad \rho(\mathcal{F}) = \text{const} \tag{3}$$

$$\textit{trace constraint:} \qquad \int_{\mathcal{F}} \mathrm{tr}(x)\, d\rho(x) = \text{const} \tag{4}$$

$$\textit{boundedness constraint:} \qquad \mathcal{T} := \iint_{\mathcal{F}\times\mathcal{F}} |xy|^2\, d\rho(x)\, d\rho(y) \leq C , \tag{5}$$

where C is a given parameter (and tr denotes the trace of a linear operator on $\mathcal{H}$).

In order to make the causal action principle mathematically well-defined, one needs to specify the class of measures in which to vary ρ. To this end, on $\mathcal{F}$ we consider the topology induced by the operator norm

$$\|A\| := \sup \left\{ \|Au\|_{\mathcal{H}} \text{ with } \|u\|_{\mathcal{H}} = 1 \right\} . \tag{6}$$

In this topology, the Lagrangian as well as the integrands in (4) and (5) are continuous. The σ-algebra generated by the open sets of $\mathcal{F}$ consists of the so-called Borel sets. A *regular Borel measure* is a measure on the Borel sets with the property that it is continuous under approximations by compact sets from inside and by open sets from outside (for basics see for example [30, §52]). The right prescription is to vary ρ within the class of regular Borel measures of $\mathcal{F}$. In the so-called *finite-dimensional setting* when $\mathcal{H}$ is finite-dimensional and the total volume $\rho(\mathcal{F})$ is finite, the existence of minimizers is proven in [9, 10], and the properties of minimizing measures are analyzed in [1, 26].

The causal action principle also makes mathematical sense in the so-called *infinite-dimensional setting* when $\mathcal{H}$ is infinite-dimensional and the total volume $\rho(\mathcal{F})$ is infinite. In this case, the volume constraint (3) is implemented by demanding that all variations $(\rho(\tau))_{\tau \in (-\varepsilon, \varepsilon)}$ should for all $\tau, \tau' \in (-\varepsilon, \varepsilon)$ satisfy the conditions

$$\big|\rho(\tau) - \rho(\tau')\big|(\mathcal{F}) < \infty \qquad \text{and} \qquad \big(\rho(\tau) - \rho(\tau')\big)(\mathcal{F}) = 0 \tag{7}$$

(where $|.|$ denotes the total variation of a measure; see [30, §28]). The existence theory in the infinite-dimensional setting has not yet been developed. But it is known that the Euler-Lagrange equations corresponding to the causal action principle still have a mathematical meaning (as will be explained in Sect. 4.1 below). This makes it possible to analyze the causal action principle without restrictions on the dimension of $\mathcal{H}$ nor on the total volume. One way of getting along without an existence theory in the infinite-dimensional setting is to take the point of view that on a fundamental physical level, the Hilbert space $\mathcal{H}$ is finite-dimensional, whereas the infinite-dimensional setting merely is a mathematical idealization needed in order to describe systems involving an infinite number of quantum particles.

We finally explain the significance of the constraints. Generally speaking, the constraints (3), (4), and (5) are needed to avoid trivial minimizers and in order for the variational principle to be well-posed. More specifically, if we dropped the constraint of fixed total volume (3), the measure $\rho = 0$ would be trivial minimizer. Without the boundedness constraint (5), the loss of compactness discussed in [10, Section 2.2] implies that no minimizers exist. If, on the other hand, we dropped the trace constraint (4), a trivial minimizer could be constructed as follows. We let x be the operator with the matrix representation

$$x = \text{diag}\big(\underbrace{1, \ldots, 1}_{n \text{ times}}, \underbrace{-1, \ldots, -1}_{n \text{ times}}, 0, 0, \ldots\big)$$

and choose ρ as a multiple of the Dirac measure supported at x. Then $\mathcal{T} > 0$ but $\mathcal{S} = 0$.

1.2 Space-Time and Causal Structure

A causal fermion system $(\mathcal{H}, \mathcal{F}, \rho)$ encodes a large amount of information. In order to recover this information, one can for example form products of linear operators in $\mathcal{F}$, compute the eigenvalues of such operator products and integrate expressions involving these eigenvalues with respect to the universal measure. However, it is not obvious what all this information means. In order to clarify the situation, we now introduce additional mathematical objects. These objects are *inherent* in the sense that we only use information already encoded in the causal fermion system.

We first define *space-time*, denoted by M, as the support of the universal measure,

$$M := \operatorname{supp} \rho \subset \mathcal{F}\,.$$

On M we consider the topology induced by $\mathcal{F}$ (generated by the sup-norm (6) on $\mathrm{L}(\mathcal{H})$). Moreover, the universal measure $\rho|_M$ restricted to M can be regarded as a volume measure on space-time. This makes space-time into a *topological measure space*. Furthermore, one has the following notion of causality:

Definition 1.2 (causal structure) For any $x, y \in \mathcal{F}$, the product xy is an operator of rank at most $2n$. We denote its non-trivial eigenvalues (counting algebraic multiplicities) by $\lambda_1^{xy}, \ldots, \lambda_{2n}^{xy}$. The points x and y are called *spacelike* separated if all the λ_j^{xy} have the same absolute value. They are said to be *timelike* separated if the λ_j^{xy} are all real and do not all have the same absolute value. In all other cases (i.e. if the λ_j^{xy} are not all real and do not all have the same absolute value), the points x and y are said to be *lightlike* separated.

Restricting the causal structure of $\mathcal{F}$ to M, we get causal relations in space-time. To avoid confusion, we remark that in earlier papers (see [14, 17]) a slightly different definition of the causal structure was used. But the modified definition used here seems preferable.

The Lagrangian (1) is compatible with the above notion of causality in the following sense. Suppose that two points $x, y \in \mathcal{F}$ are spacelike separated. Then the eigenvalues λ_i^{xy} all have the same absolute value. Rewriting (1) as

$$\mathcal{L} = \sum_{i=1}^{2n} |\lambda_i^{xy}|^2 - \frac{1}{2n} \sum_{i,j=1}^{2n} |\lambda_i^{xy}|\, |\lambda_j^{xy}| = \frac{1}{4n} \sum_{i,j=1}^{2n} \Big(|\lambda_i^{xy}| - |\lambda_j^{xy}| \Big)^2 ,$$

one concludes that the Lagrangian vanishes. Thus pairs of points with spacelike separation do not enter the action. This can be seen in analogy to the usual notion of causality where points with spacelike separation cannot influence each other.[1] This analogy is the reason for the notion "causal" in "causal fermion system" and "causal action principle."

The above notion of causality is *symmetric* in x and y, as we now explain. Since the trace is invariant under cyclic permutations, we know that

$$\operatorname{tr}\big((xy)^p\big) = \operatorname{tr}\big(x\,(yx)^{p-1}\,y\big) = \operatorname{tr}\big((yx)^{p-1}\,yx\big) = \operatorname{tr}\big((yx)^p\big) \tag{8}$$

(where tr again denotes the trace of a linear operator on $\mathcal{H}$). Since all our operators have finite rank, there is a finite-dimensional subspace I of $\mathcal{H}$ such that xy maps I

[1] For clarity, we point out that our notion of causality does allow for nonlocal correlations and entanglement between regions with space-like separation. This will become clear in Sects. 1.4 and 5.3.

to itself and vanishes on the orthogonal complement of I. Then the non-trivial eigenvalues of the operator product xy are given as the zeros of the characteristic polynomial of the restriction $xy|_I : I \to I$. The coefficients of this characteristic polynomial (like the trace, the determinant, etc.) are symmetric polynomials in the eigenvalues and can therefore be expressed in terms of traces of powers of xy. As a consequence, the identity (8) implies that the operators xy and yx have the same characteristic polynomial and are thus isospectral. This shows that the causal notions are indeed symmetric in the sense that x and y are spacelike separated if and only if y and x are (and similarly for timelike and lightlike separation). One also sees that the Lagrangian $\mathcal{L}(x, y)$ is symmetric in its two arguments.

A causal fermion system also distinguishes a *direction of time*. To this end, we let π_x be the orthogonal projection in $\mathcal{H}$ on the subspace $x(\mathcal{H}) \subset \mathcal{H}$ and introduce the functional

$$\mathcal{C} : M \times M \to \mathbb{R}, \qquad \mathcal{C}(x, y) := i \operatorname{Tr}\left(y\, x\, \pi_y\, \pi_x - x\, y\, \pi_x\, \pi_y\right) \tag{9}$$

(this functional was first stated in [18, Section 7.5], motivated by constructions in [14, Section 3.5]). Obviously, this functional is anti-symmetric in its two arguments. This makes it possible to introduce the notions

$$\begin{cases} y \text{ lies in the } \textit{future} \text{ of } x & \text{if } \mathcal{C}(x, y) > 0 \\ y \text{ lies in the } \textit{past} \text{ of } x & \text{if } \mathcal{C}(x, y) < 0\,. \end{cases} \tag{10}$$

By distinguishing a direction of time, we get a structure similar to a causal set (see for example [3]). But in contrast to a causal set, our notion of "lies in the future of" is not necessarily transitive. This corresponds to our physical conception that the transitivity of the causal relations could be violated both on the cosmological scale (there might be closed timelike curves) and on the microscopic scale (there seems no compelling reason why the causal relations should be transitive down to the Planck scale). This is the reason why we consider other structures (namely the universal measure and the causal action principle) as being more fundamental. In our setting, causality merely is a derived structure encoded in the causal fermion system.

1.3 The Kernel of the Fermionic Projector

The causal action principle depends crucially on the eigenvalues of the operator product xy with $x, y \in \mathcal{F}$. For computing these eigenvalues, it is convenient not to consider this operator product on the (possibly infinite-dimensional) Hilbert space $\mathcal{H}$, but instead to restrict attention to a finite-dimensional subspace of $\mathcal{H}$, chosen such that the operator product vanishes on the orthogonal complement of this subspace. This construction leads us to the spin spaces and to the kernel of the fermionic projector, which we now introduce. For every $x \in \mathcal{F}$ we define the

spin space S_x by $S_x = x(\mathcal{H})$; it is a subspace of $\mathcal{H}$ of dimension at most $2n$. For any $x, y \in M$ we define the *kernel of the fermionic operator* $P(x,y)$ by

$$P(x,y) = \pi_x\, y|_{S_y} \;:\; S_y \to S_x \tag{11}$$

(where π_x is again the orthogonal projection on the subspace $x(\mathcal{H}) \subset \mathcal{H}$). Taking the trace of (11) in the case $x = y$, one finds that

$$\mathrm{tr}(x) = \mathrm{Tr}_{S_x}(P_\tau(x,x))\,,$$

making it possible to express the integrand of the trace constraint (4) in terms of the kernel of the fermionic operator. In order to also express the eigenvalues of the operator xy, we define the *closed chain* A_{xy} as the product

$$A_{xy} = P(x,y)\,P(y,x) \;:\; S_x \to S_x\,. \tag{12}$$

Computing powers of the closed chain, one obtains

$$A_{xy} = (\pi_x y)(\pi_y x)|_{S_x} = \pi_x\, yx|_{S_x}\,, \qquad (A_{xy})^p = \pi_x\,(yx)^p|_{S_x}\,.$$

Taking the trace, one sees in particular that $\mathrm{Tr}_{S_x}(A_{xy}^p) = \mathrm{tr}\big((yx)^p\big)$. Repeating the arguments after (8), one concludes that the eigenvalues of the closed chain coincide with the non-trivial eigenvalues $\lambda_1^{xy}, \ldots, \lambda_{2n}^{xy}$ of the operator xy in Definition 1.2. Therefore, the kernel of the fermionic operator encodes the causal structure of M. The main advantage of working with the kernel of the fermionic operator is that the closed chain (12) is a linear operator on a vector space of dimension at most $2n$, making it possible to compute the $\lambda_1^{xy}, \ldots, \lambda_{2n}^{xy}$ as the eigenvalues of a finite matrix.

Next, it is very convenient to arrange that the kernel of the fermionic operator is symmetric in the sense that

$$P(x,y)^* = P(y,x)\,. \tag{13}$$

To this end, one chooses on the spin space S_x the *spin scalar product* $\prec .|. \succ_x$ by

$$\prec u|v\succ_x = -\langle u|xu\rangle_{\mathcal{H}} \qquad (\text{for all } u, v \in S_x)\,. \tag{14}$$

Due to the factor x on the right, this definition really makes the kernel of the fermionic operator symmetric, as is verified by the computation

$$\begin{aligned} \prec u \,|\, P(x,y)\, v\succ_x &= -\langle u \,|\, x\,P(x,y)\, v\rangle_{\mathcal{H}} = -\langle u \,|\, xy\, v\rangle_{\mathcal{H}} \\ &= -\langle \pi_y\, x\, u \,|\, y\, v\rangle_{\mathcal{H}} = \prec P(y,x)\, u \,|\, v\succ_y \end{aligned}$$

(where $u \in S_x$ and $v \in S_y$). The spin space $(S_x, \prec.|.\succ_x)$ is an *indefinite* inner product of signature (p, q) with $p, q \leq n$. In this way, indefinite inner product spaces arise naturally when analyzing the mathematical structure of the causal action principle.

The kernel of the fermionic operator as defined by (11) is also referred to as the kernel of the *fermionic projector*, provided that suitable normalization conditions are satisfied. Different normalization conditions have been proposed and analyzed (see the discussion in [28, Section 2.2]). More recently, it was observed in [20] that one of these normalization conditions is automatically satisfied if the universal measure is a minimizer of the causal action principle (see Sect. 4.2 below). With this in mind, we no longer need to be so careful about the normalization. For notational simplicity, we always refer to $P(x, y)$ as the kernel of the fermionic projector.

1.4 Wave Functions and Spinors

For clarity, we sometimes denote the spin space S_x at a space-time point $x \in M$ by S_xM. A *wave function* ψ is defined as a function which to every $x \in M$ associates a vector of the corresponding spin space,

$$\psi \;:\; M \to \mathcal{H} \qquad \text{with} \qquad \psi(x) \in S_xM \quad \text{for all } x \in M\,. \tag{15}$$

We now want to define what we mean by *continuity* of a wave function. For the notion of continuity, we need to compare the wave function at different space-time points, being vectors $\psi(x) \in S_xM$ and $\psi(y) \in S_y\mathrm{M}$ in different spin spaces. Using that both spin spaces S_xM and S_yM are subspaces of the same Hilbert space $\mathcal{H}$, an obvious idea is to simply work with the Hilbert space norm $\|\psi(x) - \psi(y)\|_{\mathcal{H}}$. However, in view of the factor x in the spin scalar product (14), it is preferable to insert a corresponding power of the operator x. Namely, the natural norm on the spin space $(S_x, \prec.|.\succ_x)$ is given by

$$\big|\psi(x)\big|_x^2 := \big\langle \psi(x) \,\big|\, |x|\, \psi(x) \big\rangle_{\mathcal{H}} = \Big\| \sqrt{|x|}\, \psi(x) \Big\|_{\mathcal{H}}^2$$

(where $|x|$ is the absolute value of the symmetric operator x on $\mathcal{H}$, and $\sqrt{|x|}$ the square root thereof). This leads us to defining that the wave function ψ is *continuous* at x if for every $\varepsilon > 0$ there is $\delta > 0$ such that

$$\Big\| \sqrt{|y|}\, \psi(y) - \sqrt{|x|}\, \psi(x) \Big\|_{\mathcal{H}} < \varepsilon \qquad \text{for all } y \in M \text{ with } \|y - x\| \leq \delta\,.$$

Likewise, ψ is said to be continuous on M if it continuous at every $x \in M$. We denote the set of continuous wave functions by $C^0(M, SM)$. Clearly, the space of continuous wave functions is a complex vector space with pointwise operations, i.e. $(\alpha\psi + \beta\phi)(x) := \alpha\psi(x) + \beta\phi(x)$ with $\alpha, \beta \in \mathbb{C}$.

It is an important observation that every vector $u \in \mathcal{H}$ of the Hilbert space gives rise to a unique wave function. To obtain this wave function, denoted by ψ^u, we simply project the vector u to the corresponding spin spaces,

$$\psi^u \;:\; M \to \mathcal{H}\,, \qquad \psi^u(x) = \pi_x u \in S_x M\,. \tag{16}$$

We refer to ψ^u as the *physical wave function* of $u \in \mathcal{H}$. The estimate[2]

$$\begin{aligned} \Big\| \sqrt{|y|}\, \psi^u(y) - \sqrt{|x|}\, \psi^u(x) \Big\|_{\mathcal{H}} &= \Big\| \sqrt{|y|}\, u - \sqrt{|x|}\, u \Big\|_{\mathcal{H}} \\ &\leq \Big\| \sqrt{|y|} - \sqrt{|x|} \Big\|\, \|u\|_{\mathcal{H}} \overset{(\star)}{\leq} \|y-x\|^{\frac{1}{4}}\, \|y+x\|^{\frac{1}{4}}\, \|u\|_{\mathcal{H}} \end{aligned}$$

shows that ψ^u is indeed continuous. The physical picture is that the physical wave functions ψ^u are those wave functions which are realized in the physical system. Using a common physical notion, one could say that the vectors in $\mathcal{H}$ correspond to the "occupied states" of the system, and that an occupied state $u \in \mathcal{H}$ is represented in space-time by the corresponding physical wave function ψ^u. The shortcoming of this notion is that an "occupied state" is defined only for free quantum fields, whereas the physical wave functions are defined also in the interacting theory. For this reason, we prefer not use the notion of "occupied states."

For a convenient notation, we also introduce the *wave evaluation operator* Ψ as an operator which to every Hilbert space vector associates the corresponding

[2]For completeness, we derive the inequality $(\star)$: Since the operator $\sqrt{|y|} - \sqrt{|x|}$ is symmetric and has finite rank, there is a normalized vector $u \in \mathcal{H}$ such that

$$\Big(\sqrt{|y|} - \sqrt{|x|} \Big) u = \pm \Big\| \sqrt{|y|} - \sqrt{|x|} \Big\|\, u\,. \tag{17}$$

Possibly by exchanging the roles of x and y we can arrange the plus sign. Then

$$\Big\| \sqrt{|y|} - \sqrt{|x|} \Big\| = \langle u \,|\, \Big(\sqrt{|y|} - \sqrt{|x|} \Big) u \rangle \leq \langle u \,|\, \Big(\sqrt{|y|} + \sqrt{|x|} \Big) u \rangle\,,$$

where in the last step we used that the operator $\sqrt{|x|}$ is positive. Multiplying by $\big\| \sqrt{|y|} - \sqrt{|x|} \big\|$ and using (17) with the plus sign, we obtain

$$\begin{aligned} &\Big\| \sqrt{|y|} - \sqrt{|x|} \Big\|^2 \\ &\leq \frac{1}{2} \Big(\langle u \,|\, \Big(\sqrt{|y|} + \sqrt{|x|} \Big) \Big(\sqrt{|y|} - \sqrt{|x|} \Big) u \rangle + \langle \Big(\sqrt{|y|} - \sqrt{|x|} \Big) u \,|\, \Big(\sqrt{|y|} + \sqrt{|x|} \Big) u \rangle \Big) \\ &= \frac{1}{2} \langle u \,|\, \Big\{ \Big(\sqrt{|y|} + \sqrt{|x|} \Big), \Big(\sqrt{|y|} - \sqrt{|x|} \Big) \Big\}\, u \rangle = \langle u \,|\, \big(|y| - |x| \big)\, u \rangle \leq \big\| |y| - |x| \big\|\,. \end{aligned}$$

We thus obtain the inequality $\big\| \sqrt{|y|} - \sqrt{|x|} \big\|^2 \leq \big\| |y| - |x| \big\|$. Applying this inequality with x replaced by x^2 and y replaced by y^2, it also follows that $\big\| |y| - |x| \big\|^2 \leq \big\| y^2 - x^2 \big\| \leq \big\| y - x \big\|\, \big\| y + x \big\|$. Combining these inequalities gives $(\star)$.

physical wave function,

$$\Psi \;:\; \mathcal{H} \to C^0(M, SM)\,, \qquad u \mapsto \psi^u\,. \tag{18}$$

Evaluating at a fixed space-time point gives the mapping

$$\Psi(x) \;:\; \mathcal{H} \to S_xM\,, \qquad u \mapsto \psi^u(x)\,.$$

The kernel of the fermionic projector can be expressed in terms of the wave evaluation operator:

Lemma 1.3 *For any $x, y \in M$,*

$$x = -\Psi(x)^*\, \Psi(x) \tag{19}$$

$$P(x,y) = -\Psi(x)\, \Psi(y)^*\,. \tag{20}$$

Proof For any $v \in S_xM$ and $u \in \mathcal{H}$,

$$\prec v \,|\, \Psi(x)\, u \succ_x \;=\; \prec v \,|\, \pi_x\, u \succ_x \;\overset{(14)}{=}\; -\langle v \,|\, x\, u \rangle_{\mathcal{H}} \;=\; \langle (-x)\, v \,|\, u \rangle_{\mathcal{H}}$$

and thus

$$\Psi(x)^* = -x|_{S_xM} \;:\; S_xM \to \mathcal{H}\,.$$

Hence

$$\Psi(x)^*\, \Psi(x)\, u = \Psi(x)^*\, \psi^u_x = -x\, \psi^u_x \overset{(16)}{=} -x\, \pi_x u = -xu\,,$$

proving (19). Similarly, the relation (20) follows from the computation

$$\Psi(x)\, \Psi(y)^* = -\pi_x\, y|_{S_y} = -P(x,y)\,.$$

This completes the proof. □

The structure of the wave functions (15) taking values in the spin spaces is reminiscent of sections of a vector bundle. The only difference is that our setting is more general in that the base space M does not need to be a manifold, and the fibres S_xM do not need to depend smoothly on the base point x. However, comparing to the setting of spinors in Minkowski space or on a Lorentzian manifold, one important structure is missing: we have no Dirac matrices and no notion of Clifford multiplication. The following definition is a step towards introducing these additional structures.

Definition 1.4 (Clifford subspace) We denote the space of symmetric linear operators on $(S_x, \prec .|. \succ_x)$ by $\mathrm{Symm}(S_x) \subset \mathrm{L}(S_x)$. A subspace $K \subset \mathrm{Symm}(S_x)$ is

called a *Clifford subspace* of signature (r, s) at the point x (with $r, s \in \mathbb{N}_0$) if the following conditions hold:

(i) For any $u, v \in K$, the anti-commutator $\{u, v\} \equiv uv + vu$ is a multiple of the identity on S_x.
(ii) The bilinear form $\langle ., . \rangle$ on K defined by

$$\frac{1}{2} \{u, v\} = \langle u, v \rangle \, \mathbb{1} \qquad \text{for all } u, v \in K \tag{21}$$

is non-degenerate and has signature (r, s).

In view of the anti-commutation relations (21), a Clifford subspace can be regarded as a generalization of the space spanned by the usual Dirac matrices. However, the above definition has two shortcomings: First, there are many different Clifford subspaces, so that there is no unique notion of Clifford multiplication. Second, we are missing the structure of tangent vectors as well as a mapping which would associate a tangent vector to an element of the Clifford subspace.

These shortcomings can be overcome by using either geometric or measure-theoretic methods. In the geometric approach, one gets along with the non-uniqueness of the Clifford subspaces by working with suitable equivalence classes. Using geometric information encoded in the causal fermion system, one can then construct mappings between the equivalence classes at different space-time points. This method will be outlined in Sect. 1.6. In the measure-theoretic approach, on the other hand, one uses the local form of the universal measure with the aim of constructing a unique Clifford subspace at every space-time point. This will be outlined in Sect. 1.7. Before entering these geometric and measure-theoretic constructions, we introduce additional structures on the space of wave functions.

1.5 The Fermionic Projector on the Krein Space

The space of wave functions can be endowed with an inner product and a topology. The inner product is defined by

$$<\psi | \phi> = \int_M \prec \psi(x) | \phi(x) \succ_x d\rho(x) \,. \tag{22}$$

In order to ensure that the last integral converges, we also introduce the scalar product $\langle\!\langle .|. \rangle\!\rangle$ by

$$\langle\!\langle \psi | \phi \rangle\!\rangle = \int_M \langle \psi(x) | \, |x| \, \phi(x) \rangle_{\mathcal{H}} \, d\rho(x) \tag{23}$$

(where $|x|$ is again the absolute value of the symmetric operator x on $\mathcal{H}$). The *one-particle space* $(\mathcal{K}, <.|.>)$ is defined as the space of wave functions for which the corresponding norm $|||\,.\,|||$ is finite, with the topology induced by this norm, and endowed with the inner product $<.|.>$. Such an indefinite inner product space with a topology induced by an additional scalar product is referred to as a *Krein space* (see for example [2, 32]).

When working with the one-particle Krein space, one must keep in mind that the physical wave function ψ^u of a vector $u \in \mathcal{H}$ does not need to be a vector in $\mathcal{K}$ because the corresponding integral in (22) may diverge. Similarly, the scalar product $\langle\!\langle \psi^u | \psi^u \rangle\!\rangle$ may be infinite. One could impose conditions on the causal fermion system which ensure that the integrals in (22) and (23) are finite for all physical wave functions. Then the mapping $u \mapsto \psi^u$ would give rise to an embedding $\mathcal{H} \hookrightarrow \mathcal{K}$ of the Hilbert space $\mathcal{H}$ into the one-particle Krein space. However, such conditions seem too restrictive and are not really needed. Therefore, here we shall not impose any conditions on the causal fermion systems but simply keep in mind that the physical wave functions are in general no Krein vectors.

Despite this shortcoming, the Krein space is useful because the kernel of the fermionic projector gives rise to an operator on $\mathcal{K}$. Namely, choosing a suitable dense domain of definition[3] $\mathcal{D}(P)$, we can regard $P(x,y)$ as the integral kernel of a corresponding operator P,

$$P \,:\, \mathcal{D}(P) \subset \mathcal{K} \to \mathcal{K}\,, \qquad (P\psi)(x) = \int_M P(x,y)\, \psi(y)\, d\rho(y)\,, \tag{24}$$

referred to as the *fermionic projector*. The fermionic projector has the following two useful properties:

- P is *symmetric* in the sense that $<P\psi|\phi> = <\psi|P\phi>$ for all $\psi, \phi \in \mathcal{D}(P)$:
  The symmetry of the kernel of the fermionic projector (13) implies that

$$\prec P(x,y)\psi(y) \,|\, \psi(x) \succ_x = \prec \psi(y) \,|\, P(y,x)\psi(x) \succ_y .$$

  Integrating over x and y and applying (24) and (22) gives the result.
- $(-P)$ is *positive* in the sense that $<\psi|(-P)\psi> \geq 0$ for all $\psi \in \mathcal{D}(P)$:
  This follows immediately from the calculation

$$<\psi|(-P)\psi> = -\iint_{M\times M} \prec \psi(x) \,|\, P(x,y)\, \psi(y) \succ_x d\rho(x)\, d\rho(y)$$

[3] For example, one may choose $\mathcal{D}(P)$ as the set of all vectors $\psi \in \mathcal{K}$ satisfying the conditions

$$\phi := \int_M x\, \psi(x)\, d\rho(x) \;\in\; \mathcal{H} \qquad \text{and} \qquad |||\,\phi\,||| < \infty\,.$$

$$= \iint_{M \times M} \langle \psi(x) \,|\, x\, \pi_x\, y\, \psi(y) \rangle_{\mathcal{H}}\, d\rho(x)\, d\rho(y) = \langle \phi | \phi \rangle_{\mathcal{H}} \geq 0\,,$$

where we again used (22) and (11) and set

$$\phi = \int_M x\, \psi(x)\, d\rho(x)\,.$$

1.6 Geometric Structures

A causal fermion system also encodes geometric information on space-time. More specifically, in the paper [14] notions of connection and curvature are introduced and analyzed. We now outline a few constructions from this paper. Recall that the kernel of the fermionic projector (11) is a mapping from one spin space to another, thereby inducing relations between different space-time points. The idea is to use these relations for the construction of a spin connection $D_{x,y}$, being a unitary mapping between the corresponding spin spaces,

$$D_{x,y} \,:\, S_y \to S_x$$

(we consistently use the notation that the subscript $_{xy}$ denotes an object at the point x, whereas the additional comma $_{x,y}$ denotes an operator which maps an object at y to an object at x). The simplest method for constructing the spin connection would be to form a polar decomposition, $P(x,y) = A_{xy}^{-\frac{1}{2}}\, U$, and to introduce the spin connection as the unitary part, $D_{x,y} = U$. However, this method is too naive, because we want the spin connection to be compatible with a corresponding metric connection $\nabla_{x,y}$ which should map Clifford subspaces at x and y (see Definition 1.4 above) isometrically to each other. A complication is that, as discussed at the end of Sect. 1.4, the Clifford subspaces at x and y are not unique. The method to bypass these problems is to work with several Clifford subspaces and to use so-called splice maps, as we now briefly explain.

First, it is useful to restrict the freedom in choosing the Clifford subspaces with the following construction. Recall that for any $x \in M$, the operator $(-x)$ on $\mathcal{H}$ has at most n positive and at most n negative eigenvalues. We denote its positive and negative spectral subspaces by S_x^+ and S_x^-, respectively. In view of (14), these subspaces are also orthogonal with respect to the spin scalar product,

$$S_x = S_x^+ \oplus S_x^-\,.$$

We introduce the *Euclidean sign operator* s_x as a symmetric operator on S_x whose eigenspaces corresponding to the eigenvalues ± 1 are the spaces S_x^+ and S_x^-, respectively. Since $s_x^2 = \mathbb{1}$, the span of the Euclidean sign operator is a one-

dimensional Clifford subspace of signature $(1, 0)$. The idea is to extend s_x to obtain higher-dimensional Clifford subspaces. We thus define a *Clifford extension* as a Clifford subspace which contains s_x. By restricting attention to Clifford extensions, we have reduced the freedom in choosing Clifford subspaces. However, there is still not a unique Clifford extension, even for fixed dimension and signature. But one can define the *tangent space* T_x as an equivalence class of Clifford extensions; for details see [14, Section 3.1]. The bilinear form $\langle ., . \rangle$ in (21) induces a Lorentzian metric on the tangent space.

Next, for our constructions to work, we need to assume that the points x and y are both regular and are properly timelike separated, defined as follows:

Definition 1.5 A space-time point $x \in M$ is said to be *regular* if x has the maximal possible rank, i.e. $\dim x(\mathcal{H}) = 2n$. Otherwise, the space-time point is called *singular*.

In most situations of physical interest (like Dirac see configurations to be discussed in Sects. 2 and 5 below), all space-time points are regular. Singular points, on the other hand, should be regarded as exceptional points or "singularities" of space-time.

Definition 1.6 The space-time points $x, y \in M$ are *properly timelike* separated if the closed chain A_{xy}, (12), has a strictly positive spectrum and if all eigenspaces are definite subspaces of $(S_x, \prec.|.\succ_x)$.

By a definite subspace of S_x we mean a subspace on which the inner product $\prec.|.\succ_x$ is either positive or negative definite.

The two following observations explain why the last definition makes sense:

- Properly timelike separation implies timelike separation (according to Definition 1.2):

  Before entering the proof, we give a simple counter example which shows why the assumption of definite eigenspaces in Definition 1.6 is necessary for the implication to hold. Namely, if the point x is regular and A_{xy} is the identity, then the eigenvalues $\lambda_1, \ldots, \lambda_{2n}$ are all strictly positive, but they are all equal.

  If $I \subset S_x$ is a definite invariant subspace of A_{xy}, then the restriction $A_{xy}|_I$ is a symmetric operator on the Hilbert space $(I, \pm \prec.|.\succ_{I \times I})$, which is diagonalizable with real eigenvalues. Moreover, the orthogonal complement $I^\perp$ of $I \subset S_x$ is again invariant. If $I^\perp$ is non-trivial, the restriction $A_{xy}|_{I^\perp}$ has at least one eigenspace. Therefore, the assumption in Definition 1.6 that all eigenspaces are definite makes it possible to proceed inductively to conclude that the operator A_{xy} is diagonalizable and has real eigenvalues.

  If x and y are properly timelike separated, then its eigenvalues are by definition all real and positive. Thus it remains to show that they are not all the same. If conversely they were all the same, i.e. $\lambda_1 = \cdots = \lambda_{2n} = \lambda > 0$, then S_x would necessarily have the maximal dimension $2n$. Moreover, the fact that A_{xy} is diagonalizable implies that A_{xy} would be a multiple of the identity on S_x.

Therefore, the spin space $(S_x, \prec.|.\succ)$ would have to be definite, in contradiction to the fact that it has signature (n, n).

- The notion is symmetric in x and y:
  Suppose that $A_{xy}u = \lambda u$ with $u \in S_x$ and $\lambda \in \mathbb{R} \setminus \{0\}$. Then the vector $w := P(y,x)\, u \in S_y$ is an eigenvector of A_{yx} again to the eigenvalue λ,

$$\begin{aligned} A_{yx}\, w &= P(y,x) P(x,y)\, P(y,x)\, u \\ &= P(y,x)\, A_{xy}\, u = \lambda\, P(y,x)\, u = \lambda w\,. \end{aligned}$$

  Moreover, the calculation

$$\begin{aligned} \lambda \prec u|u\succ &= \prec u|A_{xy}u\succ = \prec u \,|\, P(x,y)\, P(y,x)\, u\succ \\ &= \prec P(y,x)u \,|\, P(y,x)u\succ = \prec w|w\succ \end{aligned}$$

  shows that w is a definite vector if and only if u is. We conclude that A_{yx} has positive eigenvalues and definite eigenspaces if and only if A_{xy} has these properties.

So far, the construction of the spin connection has been worked out only in the case of spin dimension $n = 2$. Then for two regular and properly timelike separated points $x, y \in M$, the spin space S_x can be decomposed uniquely into an orthogonal direct sum $S_x = I^+ \oplus I^-$ of a two-dimensional positive definite subspace I^+ and a two-dimensional negative definite subspace I^- of A_{xy}. We define the *directional sign operator* v_{xy} of A_{xy} as the unique operator with eigenvalues $-1, 1, 0$ such that the eigenspaces corresponding to the eigenvalues ± 1 are the subspaces $I^\pm$.

Having the Euclidean sign operator s_x and the directional sign operator v_{xy} to our disposal, under generic assumptions one can distinguish two Clifford subspaces at the point x: a Clifford subspace K_{xy} containing v_{xy} and a Clifford extension $K_x^{(y)}$ (for details see [14, Lemma 3.12]). Similarly, at the point y we have a distinguished Clifford subspace K_{yx} (which contains v_{yx}) and a distinguished Clifford extension $K_y^{(x)}$. For the construction of the *spin connection* $D_{x,y} : S_y \to S_x$ one works with the Clifford subspaces K_{xy} and K_{yx} and demands that these are mapped to each other. More precisely, the spin connection is uniquely characterized by the following properties (see [14, Theorem 3.20]):

(i) $D_{x,y}$ is of the form

$$D_{x,y} = e^{i\varphi_{xy}\, v_{xy}}\, A_{xy}^{-\frac{1}{2}}\, P(x,y) \quad \text{with} \quad \varphi_{xy} \in (-\frac{3\pi}{4}, -\frac{\pi}{2}) \cup (\frac{\pi}{2}, \frac{3\pi}{4})\,.$$

(ii) The spin connection maps the Clifford subspaces K_{xy} and K_{yx} to each other, i.e.

$$D_{y,x}\, K_{xy}\, D_{x,y} = K_{yx}\,.$$

The spin connection has the properties

$$D_{y,x} = (D_{x,y})^{-1} = (D_{x,y})^* \qquad \text{and} \qquad A_{xy} = D_{x,y}\, A_{yx}\, D_{y,x}\,.$$

All the assumptions needed for the construction of the spin connection are combined in the notion that x and y must be *spin-connectable* (see [14, Definition 3.17]). We remark that in the limiting case of a Lorentzian manifold, the points x and y are spin-connectable if they are timelike separated and sufficiently close to each other (see [14, Section 5]).

By composing the spin connection along a discrete "path" of space-time points, one obtains a "parallel transport" of spinors. When doing so, it is important to keep track of the different Clifford subspaces and to carefully transform them to each other. In order to illustrate in an example how this works, suppose that we want to compose the spin connection $D_{y,z}$ with $D_{z,x}$. As mentioned above, the spin connection $D_{z,x}$ at the point z is constructed using the Clifford subspace K_{zx}. The spin connection $D_{y,z}$, however, takes at the same space-time point z the Clifford subspace K_{zy} as reference. This entails that before applying $D_{y,z}$ we must transform from the Clifford subspace K_{zx} to the Clifford subspace K_{zy}. This is accomplished by the *splice map* $U_z^{(y|x)}$, being a uniquely defined unitary transformation of S_x with the property that

$$K_{zy} = U_z^{(y|x)}\, K_{zx} \left(U_z^{(y|x)}\right)^* .$$

The splice map must be sandwiched between the spin connections in combinations like

$$D_{y,z}\, U_z^{(y|x)}\, D_{z,x}\,.$$

In order to construct a corresponding metric connection $\nabla_{x,y}$, one uses a similar procedure to related the Clifford subspaces to corresponding Clifford extensions. More precisely, one first unitarily transform the Clifford extension $K_y^{(x)}$ to the Clifford subspace K_{yx}. Unitarily transforming with the spin connection D_{xy} gives the Clifford subspace K_{xy}. Finally, one unitarily transforms to the Clifford extension $K_x^{(y)}$. Since the Clifford extensions at the beginning and end are representatives of the corresponding tangent spaces, we thus obtain an isometry

$$\nabla_{x,y} \;:\; T_y \to T_x$$

between the tangent spaces (for details see [14, Section 3.4]).

In this setting, *curvature* is defined as usual as the holonomy of the connection. Thus the curvature of the spin connection is given by

$$\mathfrak{R}(x,y,z) = U_x^{(z|y)}\, D_{x,y}\, U_y^{(x|z)}\, D_{y,z}\, U_z^{(y|x)}\, D_{z,x} \;:\; S_x \to S_x\,,$$

and similarly for the metric connection. In [14, Sections 4 and 5] it is proven that the above notions in fact reduce to the spinorial Levi-Civita connection and the Riemannian curvature on a globally hyperbolic Lorentzian manifold if the causal fermion system is constructed by regularizing solutions of the Dirac equation (similar as will explained in the next section for the Minkowski vacuum) and the regularization is suitably removed. These results show that the notions of connection and curvature defined above indeed generalize the corresponding notions in Lorentzian spin geometry.

1.7 Topological Structures

From a mathematical perspective, causal fermion systems provide a framework for non-smooth geometries or generalized "quantum geometries." In this context, it is of interest how the topological notions on a differentiable manifold or a spin manifold generalize to causal fermion systems. Such topological questions are analyzed in [18], as we now briefly summarize.

By definition, space-time M is a topological space (see Sect. 1.2). Attaching to every space-time point $x \in M$ the corresponding spin space S_x gives the structure of a *sheaf*, making it possible to describe the topology by sheaf cohomology. If one assumes in addition that all space-time points are regular (see Definition 1.5), then all spin spaces are isomorphic, giving rise to a *topological vector bundle*.

In order to get the connection to spinor bundles, one needs the additional structure of Clifford multiplication. As explained in Sect. 1.4, the notion of a Clifford subspace (see Definition 1.4) makes it possible to define Clifford structures at every space-time point, but the definition is not unique and does not give the connection to tangent vectors of the base space. In Sect. 1.6 these shortcomings where bypassed by working with suitable equivalence classes of Clifford subspaces. From the topological point of view, the basic question is whether one can choose a representative of this equivalence class at each space-time point in such a way that the representative depends continuously on the base point. This leads to the notion of a *Clifford section* $\mathcal{C}\ell$, being a continuous mapping which to every space-time point $x \in M$ associates a corresponding Clifford subspace $\mathcal{C}\ell_x$ (for details see [18, Section 4.1]). Choosing a Clifford section leads to the structure of a so-called *topological spinor bundle*. An advantage of working with topological spinor bundles is that no notion of differentiability is required.

If M has a differentiable structure, one would like to associate a tangent vector $u \in T_xM$ to a corresponding element of the Clifford subspace $\mathcal{C}\ell_x$. This leads to the notion of a *spin structure* γ on a topological spinor bundle, being a continuous mapping which to every $x \in M$ associates a mapping $\gamma_x : T_xM \to \mathcal{C}\ell_x$. The topological obstructions for the existence of a spin structure on a topological spinor bundle generalize the spin condition on a spin manifold (for details see [18, Sections 4.2 and 4.5]).

A useful analytic tool for the construction of Clifford sections are so-called *tangent cone measures* (see [18, Section 5]). These measures make it possible to analyze the local structure of space-time in a neighborhood of a point $x \in M$ (again without any differentiability assumptions). The tangent cone measures can be used to distinguish a specific Clifford subspace $\mathcal{C}\ell_x$ and to relate $\mathcal{C}\ell_x$ to neighboring space-time points.

We close with two remarks. First, all the above constructions generalize to the *Riemannian setting* if the definition of causal fermion systems is extended to so-called *topological fermion systems* (see [18, Definition 2.1]). We thus obtain a mathematical framework to describe *spinors on singular spaces* (see [18, Sections 7 and 8] for many examples). Second, one can introduce nontrivial topological notions even for discrete space-times by constructing neighborhoods of M in $\mathcal{F}$ (using the metric structure of $\mathcal{F}$ induced by the norm on the Banach space $\mathrm{L}(\mathcal{H})$) and by studying the topology of these neighborhoods.

2 Correspondence to Minkowski Space

In order to put the abstract framework in a simple and concrete context, we now explain how to describe Dirac spinors in Minkowski space as a causal fermion system.

2.1 Concepts Behind the Construction of Causal Fermion Systems

We let $(\mathscr{M}, \langle .,. \rangle)$ be Minkowski space (with the signature convention $(+---)$) and $d\mu$ the standard volume measure (thus $d\mu = d^4x$ in a reference frame $x = (x^0, \ldots, x^3)$). We denote the spinor space at a point $x \in \mathscr{M}$ by $S_x\mathscr{M}$, so that a Dirac wave function ψ takes values in

$$\psi(x) \in S_x\mathscr{M} \simeq \mathbb{C}^4 .$$

The spinor space at x is endowed with an indefinite inner product of signature $(2, 2)$, which as in physics textbooks we denote by $\overline{\psi}\phi$ (where $\overline{\psi} = \psi^\dagger \gamma^0$ is the usual adjoint spinor). Clearly, in Minkowski space one has a trivial parallel transport of spinors, making it possible to identify the spinor spaces at different space-time points. Thus the space-time index $S_x\mathscr{M}$ of the spinor space is added only for notational clarity.

On the solutions of the Dirac equation

$$(i\gamma^j \partial_j - m)\psi = 0 \tag{25}$$

we consider the usual Lorentz invariant scalar product

$$(\psi|\phi) := 2\pi \int_{\mathbb{R}^3} (\overline{\psi}\gamma^0\phi)(t,\vec{x})\, d^3x\,, \tag{26}$$

making the solution space to a separable Hilbert space. We choose $\mathcal{H}$ as a closed subspace of this Hilbert space with the induced scalar product $\langle .|.\rangle_{\mathcal{H}} := (.|.)|_{\mathcal{H}\times\mathcal{H}}$. Clearly, $\mathcal{H}$ is again a separable Hilbert space. In order to describe the vacuum (i.e. the physical system where no particles and anti-particles are present), one chooses $\mathcal{H}$ as the subspace spanned by all the negative-energy solutions (the "Dirac sea vacuum"). To describe particles or anti-particles, one includes positive-energy solutions or leaves out negative-energy solutions, respectively. But any other closed subspace of the solution space may be chosen as well. We remark for clarity that in this section, we only consider the vacuum Dirac equation (25), so that the Dirac particles do not interact (interacting systems will be discussed in Sect. 5 below).

In order to get into the framework of causal fermion systems, to every space-time point $x \in \mathscr{M}$ we want to associate a linear operator $F(x) \in \mathcal{F}$. Once this has been accomplished, the resulting mapping

$$F \;:\; \mathscr{M} \to \mathcal{F}\,. \tag{27}$$

can be used to introduce a measure ρ on $\mathcal{F}$. Namely, we say that a subset $\Omega \subset \mathcal{F}$ is measurable if and only if its pre-image $F^{-1}(\Omega)$ is a measurable subset of $\mathscr{M}$. Moreover, we define the measure of Ω as the space-time volume of the pre-image, $\rho(\Omega) := \mu(F^{-1}(\Omega))$. This construction is commonly used in mathematical analysis and is referred to as the *push-forward measure*, denoted by

$$\rho = F_* \mu\,.$$

Then $(\mathcal{H}, \mathcal{F}, \rho)$ will be a causal fermion system.

The basic idea for constructing $F(x)$ is to represent the inner product on the spinors in terms of the Hilbert space scalar product, i.e.

$$\langle \psi | F(x) \phi \rangle_{\mathcal{H}} = -(\overline{\psi}\phi)(x) \qquad \text{for all } \psi, \phi \in \mathcal{H}\,. \tag{28}$$

The operator $F(x)$ gives information on the densities and correlations of the Dirac wave functions at the space-time point x. It is referred to as the *local correlation operator* at x. Relating the maximal number of positive and negative eigenvalues of $F(x)$ to the signature of the inner product $(\overline{\psi}\phi)(x)$, one sees that $F(x)$ indeed has at most two positive and at most two negative eigenvalues. However, Eq. (28) suffers from the shortcoming that the right side is in general ill-defined because solutions $\psi, \phi \in \mathcal{H}$ are in general not continuous and thus cannot be evaluated pointwise. This is the reason why we need to introduce an *ultraviolet regularization* (UV regularization). Before entering the analysis, we first outline our method and

explain the physical picture in a few remarks. The mathematical construction will be given afterwards in Sect. 2.2.

In order to put our constructions in the general physical context, we first note that UV regularizations are frequently used in relativistic quantum field theory as a technical tool to remove divergences. A common view is that the appearance of such divergences indicates that the physical theory is incomplete and should be replaced for very small distances by another, more fundamental theory. The renormalization program is a method to get along with standard quantum field theory by finding a way of dealing with the divergences. The first step is the UV regularization, which is usually a set of prescriptions which make divergent integrals finite. The next step of the renormalization program is to show that the UV regularization can be taken out if other parameters of the theory (like masses and coupling constants) are suitably rescaled. Conceptually, in the renormalization program the UV regularization merely is a technical tool. All predictions of theory should be independent of how the regularization is carried out.

In the context of causal fermion systems, however, the physical picture behind the UV regularization is quite different. Namely, in our setting the *regularized* objects are to be considered as the fundamental physical objects. Therefore, the regularization has a physical significance. It should describe the microscopic structure of physical space-time.

Before explaining this physical picture in more detail, we need to introduce a microscopic length scale $\varepsilon > 0$ on which the UV regularization should come into play. Regularization lengths are often associated to the Planck length $\ell_P \approx 1.6 \cdot 10^{-35}$ m. The analysis of the gravitational field in [6] suggests that ε should be chosen even much smaller than the Planck length (see [6, Section 4.9 and §5.4.3]). Even without entering a detailed discussion of the length scales, it is clear that ε will be by many orders of magnitude smaller than most other physical length scales of the system. Therefore, it is a sensible method to analyze the causal action principle in the asymptotics when ε is very small. In order to make such an asymptotics mathematically precise, we necessarily need to consider the *regularization length* ε as a *variable parameter* taking values in an interval $(0, \varepsilon_{\max})$. Only for such a variable parameter, one can analyze the asymptotics as $\varepsilon \searrow 0$.

For any $\varepsilon \in (0, \varepsilon_{\max})$, similar to (27) we shall construct a mapping $F^\varepsilon : \mathscr{M} \to \mathcal{F}$ by suitably inserting an UV regularization in (28). Then we construct the corresponding universal measure as the push-forward by F^ε, i.e.

$$\rho^\varepsilon := F^\varepsilon_* \mu \,. \tag{29}$$

This shall give rise to a causal fermion system $(\mathcal{H}, \mathcal{F}, \rho^\varepsilon)$. We will also explain how to identify the objects in Minkowski space with corresponding objects of the causal fermion system:

Minkowski space	Causal fermion system
Space-time point $x \in \mathscr{M}$	Space-time point $x \in M^\varepsilon := \operatorname{supp} \rho^\varepsilon$
Topology of $\mathscr{M}$	Topology of M^ε
Spinor space $S_x\mathscr{M}$	Spin space S_xM^ε
Causal structure of Minkowski space	Causal structure of Definition 1.2

With these identifications made, the structures of Minkowski space are no longer needed. They are encoded in the causal fermion system, and we may describe the physical space-time exclusively by the causal fermion system. We consider the objects with UV regularization as described by the causal fermion system as the fundamental physical objects.

In the following remarks we elaborate on the physical picture behind the UV regularization and explain why our setting is sufficiently general to describe the physical situation we have in mind.

Remark 2.1 (method of variable regularization) As just explained, the only reason for considering a family of causal fermion systems is to give the asymptotics $\varepsilon \searrow 0$ a precise mathematical meaning. But from the physical point of view, a specific regularization for a specific value of ε should be distinguished by the fact that the corresponding causal fermion system $(\mathcal{H}, \mathcal{F}, \rho^\varepsilon)$ describes our physical space-time. We again point out that this concept is different from standard quantum field theory, where the regularization merely is a technical tool used in order to remove divergences. In our setting, the regularization has a physical significance. The *regularized* objects are to be considered as the *fundamental* physical objects, and the regularization is a method to describe the microscopic structure of physical space-time.

This concept immediately raises the question how the "physical regularization" should look like. Generally speaking, the regularized space-time should look like Minkowski space down to distances of the scale ε. For distances smaller than ε, the structure of space-time may be completely different. The simplest method of regularizing is to "smear out" or "mollify" all wave functions on the scale ε (this corresponds to Example 2.4 below). But it is also conceivable that space-time has a non-trivial microstructure on the scale ε, which cannot be guessed or extrapolated from the structures of Minkowski space. Since experiments on the length scale ε seem out of reach, it is completely unknown what the microscopic structure of space-time is. Nevertheless, we can hope that we can get along without knowing this micro-structure, because the detailed form of this micro-structure might have no influence on the effective physical equations which are valid on the energy scales accessible to experiments. More precisely, the picture is that the general structure of the effective physical equations should be independent of the micro-structure of space-time. Values of mass ratios or coupling constants, however, may well depend on the micro-structure (a typical example is the gravitational constant, which is closely tied to the Planck length, which in turn is related to ε as explained in [6, Section 4.9]). In more general terms, the unknown micro-structure of space-

time should enter the effective physical equations only by a finite (hopefully small) number of free parameters, which can then be taken as empirical free parameters of the effective macroscopic theory.

Clearly, the above picture must be questioned and supported by mathematical results. To this end, one needs to analyze in detail how the effective macroscopic theory depends on the regularization. For this reason, it is not sufficient to consider a specific family of regularizations. Instead, one must analyze a whole class of regularizations which is so large that it covers all relevant regularization effects. This strategy is referred to as the *method of variable regularization* (for a longer explanation see [8, §4.1]). It is the reason why in Definition 2.3 below we shall only state properties of the regularization, but we do not specify how precisely it should look like. ◇

Remark 2.2 (sequences of finite-dimensional regularizations) The critical reader may wonder why we consider a family of regularizations $(\mathcal{H}, \mathcal{F}, \rho^\varepsilon)$ parametrized by a continuous parameter $(0, \varepsilon_{\max})$. Would it not be more suitable to consider instead a sequence of causal fermion systems $(\mathcal{H}_\ell, \mathcal{F}_\ell, \rho_\ell)$ which asymptotically as $\ell \to \infty$ describes Minkowski space? A related question is why we constructed the measure ρ as the push-forward of the Lebesgue measure (29). Would it not be better to work with more general measures such as to allow for the possibility of discrete micro-structures? The answer to these questions is that it is no loss of generality and a simply a matter of convenience to work with the family $(\mathcal{H}, \mathcal{F}, \rho^\varepsilon)$ with $\varepsilon \in (0, \varepsilon_{\max})$, as we now explain.

We first point out that we do not demand our family $(\mathcal{H}, \mathcal{F}, \rho^\varepsilon)$ to be in any sense "continuous" in the parameter ε. Therefore, one can also describe a sequence $(\mathcal{H}, \mathcal{F}, \rho_\ell)$ simply by choosing the family ρ^ε to be piecewise constant, for example

$$\rho^\varepsilon = \rho_\ell \qquad \text{if} \qquad \frac{1}{\ell} \leq \varepsilon < \frac{1}{\ell+1}\,.$$

Similarly, it is no loss of generality to take ρ as the push-forward measure of the Lebesgue measure because $F^\varepsilon(x)$ need not depend continuously on $x \in M$. For example, one can arrange a discrete space-time like a space-time lattice by choosing F^ε as a mapping which is piecewise constant on little cubes of Minkowski space. Clearly, this mapping is not continuous, but it is continuous almost everywhere. Moreover, its image is a discrete set, corresponding to a discrete micro-structure of space-time. For the method for representing a general measure ρ as the push-forward of for example the Lebesgue measure we refer the interested reader to the proof of [10, Lemma 1.4].

The remaining question is why we may keep the Hilbert space $\mathcal{H}$ fixed. In particular, we noted in Sect. 1.1 that the existence of minimizers of the causal action principle has been proven only if $\mathcal{H}$ is finite-dimensional. Therefore, should one not consider a filtration $\mathcal{H}_1 \subset \mathcal{H}_2 \subset \cdots \subset \mathcal{H}$ of $\mathcal{H}$ by finite-dimensional subspaces? Indeed, from the conceptual point of view, this would be the correct

way to proceed. Nevertheless, the following consideration explains why we can just as well replace all the Hilbert spaces $\mathcal{H}_\ell$ by the larger space $\mathcal{H}$: For a given causal fermion system $(\mathcal{H}_\ell, \mathcal{F}_\ell, \rho_\ell)$ with $\mathcal{H}_\ell \subset \mathcal{H}$, by extending all operators by zero to the orthogonal complement of $\mathcal{H}_\ell$, one obtains the so-called *extended causal fermion system* $(\mathcal{H}, \mathcal{F}, \rho_\ell)$. The fact that the causal fermion system was extended can still be seen by forming the so-called *effective Hilbert space* as

$$\mathcal{H}^{\text{eff}} = \overline{\text{span}\{x(\mathcal{H}) \,|\, x \in \text{supp}\, \rho\}}\,.$$

Namely, for an extended causal fermion system, the effective Hilbert space still is a subset of the original Hilbert space, $\mathcal{H}^{\text{eff}} \subset \mathcal{H}_\ell$. Moreover, the support of the extended causal fermion system is still contained in $\mathcal{F}_\ell \subset \text{L}(\mathcal{H}_\ell)$. Therefore, we do not lose any information by extending a causal fermion system. Conversely, when analyzing a causal fermion system, it seems preferable to always make the Hilbert space as small as possible by taking $\mathcal{H}^{\text{eff}}$ as the underlying Hilbert space.

The delicate point about extending causal fermion systems is that the causal action principle does depend sensitively on the dimension of the underlying Hilbert space $\mathcal{H}$. More specifically, the infimum of the action is known to be strictly decreasing in the dimension of $\mathcal{H}$ (see the estimates in [9, Lemma 5.1], which apply similarly in the more general setting of [10]). Therefore, a minimizer ρ of the causal action principle will no longer be a minimizer if the causal fermion system is extended. However, the first order *Euler-Lagrange equations* (for details see Sect. 4.1 below) are still satisfied for the extended causal fermion system. Therefore, for convenience we fix the Hilbert space $\mathcal{H}$ and consider a family of causal fermion systems $(\mathcal{H}, \mathcal{F}, \rho^\varepsilon)$ thereon. In order for the causal action principle to be well-defined and for ρ^ε to be a minimizer, one should replace $\mathcal{H}$ by the corresponding effective Hilbert space $\mathcal{H}^{\text{eff}}$, which may depend on ε and should be arranged to be finite-dimensional. For the analysis of the Euler-Lagrange equations, however, the restriction to $\mathcal{H}^{\text{eff}}$ is unnecessary, and it is preferable to work with the extended Hilbert space $\mathcal{H}$. ◇

We finally remark that the hurried reader who wants to skip the following constructions may read instead the introductory section [17, Section 1.1] where formal considerations without UV regularization are given. Moreover, a more explicit analysis of four-dimensional Minkowski space with a particularly convenient regularization is presented in [14, Section 4]. For a somewhat simpler analysis of two-dimensional Minkowski space we refer to [18, Section 7.2].

2.2 Introducing an Ultraviolet Regularization

We now enter the construction of the UV regularization. We denote the continuous Dirac wave functions (i.e. the continuous sections of the spinor bundle, not necessarily solutions of the Dirac equation) by $C^0(\mathscr{M}, S\mathscr{M})$. Similarly, the smooth wave

functions with compact support in a subset $K \subset \mathscr{M}$ are denoted by $C_0^\infty(K, S\mathscr{M})$. For the C^k-norms we use the notation

$$|\eta|_{C^k(K)} = \sum_{|\alpha| \leq k} \sup_{x \in K} |\partial^\alpha \eta(x)| \qquad \text{for } \eta \in C_0^\infty(K, S\mathscr{M}) \,,$$

where the α are multi-indices. Here $|.|$ is any pointwise norm on the spinor spaces (we again identify all spinor spaces with the trivial parallel transport). Since any two such norms can be estimated from above and below by a constant, the C^k-norms corresponding to different choices of the norms $|.|$ are also equivalent. For example, one can choose $|\psi|^2 := \overline{\psi} \gamma^0 \psi$ similar to the integrand in the scalar product (26). But clearly, other choices are possible just as well.

The UV regularization is performed most conveniently with so-called regularization operators, which we now define.

Definition 2.3 Consider a family of linear operators $(\mathfrak{R}_\varepsilon)$ with $0 < \varepsilon < \varepsilon_{\max}$ which map $\mathcal{H}$ to the continuous wave functions,

$$\mathfrak{R}_\varepsilon \,:\, \mathcal{H} \to C^0(\mathscr{M}, S\mathscr{M}) \,.$$

The family is called a family of **regularization operators** if the following conditions hold:

(i) The image of every regularization operator is pointwise bounded, meaning that for every $\varepsilon \in (0, \varepsilon_{\max})$ and all $x \in \mathscr{M}$ there is a constant $c > 0$ such that for all $u \in \mathcal{H}$,

$$\big|\big(\mathfrak{R}_\varepsilon u\big)(x)\big| \leq c\, \|u\|_{\mathcal{H}} \,. \tag{30}$$

(ii) The image of every regularization operator is equicontinuous almost everywhere in the sense that for every $\varepsilon \in (0, \varepsilon_{\max})$, almost all $x \in \mathscr{M}$ and every $\delta > 0$, there is an open neighborhood $U \subset \mathscr{M}$ of x such that for all $u \in \mathcal{H}$ and all $y \in U$,

$$\big|\big(\mathfrak{R}_\varepsilon u\big)(x) - \big(\mathfrak{R}_\varepsilon u\big)(y)\big| \leq \delta\, \|u\|_{\mathcal{H}} \,. \tag{31}$$

(iii) In the limit $\varepsilon \searrow 0$, the family converges weakly to the identity, meaning that for every compact subset $K \subset \mathscr{M}$ and every $\delta > 0$ there is a constant $\varepsilon_0 > 0$, such that for all $\varepsilon \in (0, \varepsilon_0)$, $u \in \mathcal{H}$ and $\eta \in C_0^\infty(K, S\mathscr{M})$,

$$\Big| \int_{\mathscr{M}} \overline{\eta(x)} \big(\mathfrak{R}_\varepsilon(u) - u\big)(x)\, d^4x \Big| \leq \delta\, \|u\|_{\mathcal{H}}\, |\eta|_{C^1(K)} \,. \tag{32}$$

We point out that we do not demand that the regularized wave function $\mathfrak{R}_\varepsilon \psi$ is again a solution of the Dirac equation. This could be imposed (as is done in [25,

Section 4]), but doing so seems too restrictive for the physical applications. We also note that "almost all" in (ii) refers to the standard volume measure $d\mu$ on $\mathscr{M}$.

For the mathematically interested reader we remark that the above properties (i) and (ii) are very similar to the assumptions in the Arzelà-Ascoli theorem (see for example [5, Section VII.5] or [35, Theorem 7.25]). In fact, if we replaced "almost all" in (ii) by "all", one could apply the Arzelà-Ascoli theorem and restate the properties (i) and (ii) equivalently by saying that taking the image $\mathfrak{R}_\varepsilon(B_1(0))$ of the unit ball in $\mathcal{H}$ and restricting the resulting family of functions to any compact set $K \subset \mathscr{M}$, one obtains a relatively compact subset of $C^0(K, S\mathscr{M})$. It is remarkable that the properties (i) and (ii) come up naturally as conditions for a sensible UV regularization, although we shall never use compactness arguments in our proofs. Weakening "all" by "almost all" in (ii) makes it possible to describe discrete space-times like space-time lattices, as was mentioned in Remark 2.2 above.

Simple examples of regularization operators are obtained by mollifying the wave functions on the scale ε:

Example 2.4 (regularization by mollification) Let $h \in C_0^\infty(\mathscr{M}, \mathbb{R})$ be a non-negative test function with

$$\int_{\mathscr{M}} h(x)\, d^4x = 1\,.$$

We define the operators $\mathfrak{R}_\varepsilon$ for $\varepsilon > 0$ as the convolution operators

$$(\mathfrak{R}_\varepsilon u)(x) := \frac{1}{\varepsilon^4} \int_{\mathscr{M}} h\Big(\frac{x-y}{\varepsilon}\Big)\, u(y)\, d^4y\,.$$

Let us prove that the family $(\mathfrak{R}_\varepsilon)_{0<\varepsilon<1}$ is a family of regularization operators. First,

$$\big|\big(\mathfrak{R}_\varepsilon u\big)(x)\big| \leq \frac{|h|_{C^0}}{\varepsilon^4} \int_K |u(y)|\, d^4y \leq \frac{|h|_{C^0}}{\varepsilon^4}\, \sqrt{\mu(K)}\, \Big(\int_K |u(y)|^2\, d^4y\Big)^{\frac{1}{2}}\,,$$

where in the last step we used the Schwarz inequality. We now rewrite the obtained space-time integral of $|u|^2$ with the help of Fubini's theorem as a bounded time integral and a spatial integral. In view of (26), the spatial integral can be estimated by the Hilbert space norm. We thus obtain

$$\int_K |u(y)|^2\, d^4y \leq C \int_K \big(\overline{u}\gamma^0 u\big)(y)\, d^4y \leq C \int_{t_0}^{t_1} \|u\|_{\mathcal{H}}^2 = C\,(t_1 - t_0)\, \|u\|_{\mathcal{H}}^2\,, \tag{33}$$

where t_0 and t_1 are chosen such that K is contained in the time strip $t_0 < t < t_1$. We conclude that

$$\big|\big(\mathfrak{R}_\varepsilon u\big)\big| \leq \frac{|h|_{C^0}}{\varepsilon^4}\, \sqrt{\mu(K)\, C\,(t_1 - t_0)}\, \|u\|_{\mathcal{H}}^2\,,$$

proving (30).

In order to derive the inequality (31), we begin with the estimate

$$\big|\big(\mathfrak{R}_\varepsilon u\big)(x) - \big(\mathfrak{R}_\varepsilon u\big)(y)\big| \leq \frac{1}{\varepsilon^4} \sup_{z \in \mathscr{M}} \Big| h\Big(\frac{x-z}{\varepsilon}\Big) - h\Big(\frac{y-z}{\varepsilon}\Big)\Big| \int_K |u(y)|\, d^4y\,.$$

Again applying (33) and using that h is uniformly continuous, one obtains (31).

It remains to prove (32). We first write the integral on the left as

$$\int_{\mathscr{M}} \overline{\eta(x)}\big(\mathfrak{R}_\varepsilon(u) - u\big)(x)\, d^4x = \int_{\mathscr{M}} \overline{\big(\eta_\varepsilon(y) - \eta(y)\big)}\, u(y)\, d^4y\,, \tag{34}$$

where we set

$$\eta_\varepsilon(y) = \frac{1}{\varepsilon^4} \int_{\mathscr{M}} \eta(x)\, h\Big(\frac{x-y}{\varepsilon}\Big)\, d^4x\,.$$

Now we use the standard estimate for convolutions

$$\begin{aligned} |\eta_\varepsilon(y) - \eta(y)| &= \frac{1}{\varepsilon^4} \Big| \int_{\mathscr{M}} \big(\eta(x) - \eta(y)\big)\, h\Big(\frac{x-y}{\varepsilon}\Big)\, d^4x \Big| \\ &= \Big| \int_{\mathscr{M}} \Big(\eta(y+\varepsilon z) - \eta(y)\Big)\, h(z)\, d^4z \Big| \leq |\eta|_{C^1(K)} \int_{\mathscr{M}} |\varepsilon z|\;\; h(z)\, d^4z \end{aligned}$$

(where in the last step we used the mean value theorem). This gives rise to the estimate

$$|\eta_\varepsilon - \eta|_{C^0(K)} \leq c\, \varepsilon\, |\eta|_{C^1(K)}\,,$$

where c may depend on K and the choice of h, but is independent of η. This makes it possible to estimate (34) by

$$\Big| \int_{\mathscr{M}} \overline{\eta(x)}\big(\mathfrak{R}_\varepsilon(u) - u\big)(x)\, d^4x \Big| \leq \varepsilon\, |\eta|_{C^1(K)} \int_K |u(y)|_y\, d^4y\,.$$

Again applying (33), we conclude that

$$\Big| \int_{\mathscr{M}} \overline{\eta(x)}\big(\mathfrak{R}_\varepsilon(u) - u\big)(x)\, d^4x \Big| \leq \delta\, |\eta|_{C^1(K)}\, \sqrt{\mu(K)}\, \sqrt{C\,(t_1 - t_0)}\, \|u\|_{\mathscr{H}}\,,$$

proving (32). ◇

Given a family of regularization operators, we can construct causal fermion systems as follows. We fix $\varepsilon \in (0, \varepsilon_{\max})$. For any $x \in \mathscr{M}$, we consider the bilinear form

$$b_x : \mathscr{H} \times \mathscr{H} \to \mathbb{C}\,, \quad b_x(u,v) = -\overline{(\mathfrak{R}_\varepsilon u)(x)}(\mathfrak{R}_\varepsilon v)(x)\,. \tag{35}$$

This bilinear form is well-defined and bounded because $\mathfrak{R}_\varepsilon$ is defined pointwise and because evaluation at x gives a linear operator of finite rank. Thus for any $v \in \mathcal{H}$, the anti-linear form $b_x(.,v) : \mathcal{H} \to \mathbb{C}$ is continuous. By the Fréchet-Riesz theorem (see for example [33, Section 6.3]), there is a unique vector $w \in \mathcal{H}$ such that $b_x(u,v) = \langle u|w\rangle_{\mathcal{H}}$ for all $u \in \mathcal{H}$. The mapping $v \mapsto w$ is linear and bounded. We thus obtain a bounded linear operator $F^\varepsilon(x)$ on $\mathcal{H}$ such that

$$b_x(u,v) = \langle u \,|\, F^\varepsilon(x)\, v\rangle_{\mathcal{H}} \qquad \text{for all } u, v \in \mathcal{H}\,.$$

Taking into account that the inner product on the Dirac spinors at x has signature $(2,2)$, the local correlation operator $F^\varepsilon(x)$ is a symmetric operator on $\mathcal{H}$ of rank at most four, which has at most two positive and at most two negative eigenvalues. Finally, we introduce the *universal measure* $\rho^\varepsilon = F^\varepsilon_* \mu$ as the push-forward of the volume measure on $\mathscr{M}$ under the mapping F^ε. In this way, for every $\varepsilon \in (0, \varepsilon_0)$ we obtain a causal fermion system $(\mathcal{H}, \mathcal{F}, \rho^\varepsilon)$ of spin dimension $n = 2$.

2.3 Correspondence of Space-Time

We now explain the connection between points of Minkowski space and points of space-time $M^\varepsilon := \operatorname{supp} \rho^\varepsilon$ of the corresponding causal fermion system $(\mathcal{H}, \mathcal{F}, \rho^\varepsilon)$. We begin with a general characterization of M^ε.

Proposition 2.5 *For any $\varepsilon \in (0, \varepsilon_{\max})$, there is a subset $E \subset \mathscr{M}$ of μ-measure zero such that the mapping $F^\varepsilon|_{\mathscr{M}\setminus E} : \mathscr{M} \setminus E \to \mathcal{F}$ is continuous. Moreover, the support of the universal measure $M^\varepsilon := \operatorname{supp} \rho^\varepsilon$ is given by*

$$M^\varepsilon = \overline{F^\varepsilon(\mathscr{M} \setminus E)}^{L(\mathcal{H})}\,. \tag{36}$$

Proof To show continuity, we need to estimate the sup-norm $\|F^\varepsilon(x) - F^\varepsilon(y)\|$. We first write the expectation value of the corresponding operator by

$$\begin{aligned}
&\langle u \,|\, \big(F^\varepsilon(x) - F^\varepsilon(y)\big)\, v\rangle_{\mathcal{H}} = -\overline{(\mathfrak{R}_\varepsilon\, u)(x)}(\mathfrak{R}_\varepsilon\, v)(x) + \overline{(\mathfrak{R}_\varepsilon\, u)(y)}(\mathfrak{R}_\varepsilon\, v)(y) \\
&\quad = -\overline{(\mathfrak{R}_\varepsilon\, u)(x)}\big((\mathfrak{R}_\varepsilon\, v)(x) - (\mathfrak{R}_\varepsilon\, v)(y)\big) - \overline{\big((\mathfrak{R}_\varepsilon\, u)(x) - (\mathfrak{R}_\varepsilon\, u)(y)\big)}(\mathfrak{R}_\varepsilon\, v)(y)\,,
\end{aligned}$$

giving rise to the estimate

$$\begin{aligned}
&\big|\langle u \,|\, \big(F^\varepsilon(x) - F^\varepsilon(y)\big) v\rangle_{\mathcal{H}}\big| \\
&\quad \le |(\mathfrak{R}_\varepsilon\, u)(x)|\, \big|(\mathfrak{R}_\varepsilon\, v)(x) - (\mathfrak{R}_\varepsilon\, v)(y)\big| + \big|(\mathfrak{R}_\varepsilon\, u)(x) - (\mathfrak{R}_\varepsilon\, u)(y)\big|\, |(\mathfrak{R}_\varepsilon\, v)(y)|\,.
\end{aligned}$$

We now estimate the resulting spinor norms with the help of properties (i) and (ii) of Definition 2.3. First, we denote the exceptional set of μ-measure zero where (31) does not hold by $E \subset \mathscr{M}$. Combining (30) and (31), one immediately sees that every

point $x \in \mathscr{M} \setminus E$ has a neighborhood U such that the boundedness property (30) holds uniformly on U (i.e. $|(\mathfrak{R}_\varepsilon u)(y)| \leq c\, \|u\|_{\mathscr{H}}$ for all $y \in U$). We thus obtain the estimate

$$\big|\langle u \,|\, \big(F^\varepsilon(x) - F^\varepsilon(y)\big) v\rangle_{\mathscr{H}}\big| \leq 2c\,\delta\, \|u\|_{\mathscr{H}}\, \|v\|_{\mathscr{H}}\,,$$

valid for all $y \in U$ and $u, v \in \mathscr{H}$. Hence the sup-norm is bounded by $\|F^\varepsilon(x) - F^\varepsilon(y)\| \leq 2c\delta$, showing that F^ε is continuous on $\mathscr{M} \setminus E$.

It remains to prove (36). Since $\mu(E) = 0$, the set E can be disregarded when forming the push-forward measure. Therefore, taking into account that the support of a measure is by definition a closed set, it suffices to show that for every $x \in \mathscr{M} \setminus E$, the operator $p := F^\varepsilon(x)$ lies in the support of ρ^ε. Let $U \subset \mathscr{F}$ be an open neighborhood of p. Then the continuity of F^ε at x implies that the preimage $(F^\varepsilon)^{-1}(U)$ is an open subset of $\mathscr{M}$. Hence the Lebesgue measure of this subset is non-zero, $\mu((F^\varepsilon)^{-1}(U)) > 0$. By definition of the push-forward measure, it follows that $\rho^\varepsilon(U) > 0$. Hence every neighborhood of p has a non-zero measure, implying that $p \in \operatorname{supp} \rho^\varepsilon$. This concludes the proof. □

In order to have a convenient notation, in what follows we always identify a point in Minkowski space with the corresponding operator of the causal fermion system,

$$\text{identify} \quad x \in \mathscr{M} \qquad \text{with} \qquad F^\varepsilon(x) \in \mathscr{F}\,. \tag{37}$$

In general, this identification is not one-to-one, because the mapping F^ε need not be injective. In the latter case, there are two points $x, y \in \mathscr{M}$ such that the bilinear forms b_x and b_y coincide (see (35)). In other words, all correlations between regularized wave functions coincide at the points x and y. Using a more physical language, this means that the points x, y of Minkowski space are not distinguishable by any experiments performed on the fermionic wave functions. We take the point of view that in such situations, the points x and y should not be distinguished physically, and that it is reasonable and desirable that the two points are identified in the causal fermion system with the same space-time point $F^\varepsilon(x) = F^\varepsilon(y) \in M^\varepsilon := \operatorname{supp} \rho^\varepsilon$. In philosophical terms, our construction realizes the principle of the identity of indiscernibles.

We also remark that, due to the closure in (36), it may happen that the space-time M^ε contains a point z which does *not* lie in the image of F^ε, but is merely a limit point in $F^\varepsilon(\mathscr{M})$. In this case, the corresponding bilinear form $b(u, v) := \langle u | z v\rangle_{\mathscr{H}}$ can be approximated with an arbitrarily small error by bilinear forms b_x with $x \in \mathscr{M}$. Since experiments always involve small imprecisions, we take the point of view that it is again reasonable and desirable mathematically to include z into the space-time points.

Generally speaking, the just-discussed cases that F^ε is not injective or its image is not closed seem mostly of academic interest. In most applications, the mapping F^ε will be injective and closed. In all these situations, Proposition 2.5 will give us a one-to-one correspondence between points $x \in \mathscr{M}$ and points $F^\varepsilon(x) \in M^\varepsilon$.

We finally note that, working with the push-forward measure (29), the volume measure on space-time M^ε as defined by the universal measure $d\rho^\varepsilon$ always agrees under the identification (37) with the Lebesgue measure $d\mu$ on $\mathscr{M}$.

2.4 Correspondence of Spinors and Wave Functions

We proceed by explaining the connection between the spinor space $S_x\mathscr{M}$ at a point $x \in \mathscr{M}$ of Minkowski space and the corresponding spin space $S_xM \subset \mathcal{H}$ of the causal fermion system (where we use the identification (37)). This will also make it possible to get a connection between Dirac wave functions in Minkowski space and wave functions as defined in Sect. 1.4. In preparation, we derive useful explicit formulas for the local correlation operators. To this end, for any $x \in \mathscr{M}$ we define the *evaluation map* e_x^ε by

$$e_x^\varepsilon \;:\; \mathcal{H} \to S_x\mathscr{M}, \qquad e_x^\varepsilon \psi = (\mathfrak{R}_\varepsilon \psi)(x)\,. \tag{38}$$

Its adjoint is defined as usual, taking into account the corresponding inner products on the domain and the target space, i.e.

$$\langle (e_x^\varepsilon)^* \chi \,|\, \psi \rangle_{\mathcal{H}} = \overline{\chi}\left(e_x^\varepsilon \psi\right).$$

We denote this adjoint by ι_x^ε,

$$\iota_x^\varepsilon := (e_x^\varepsilon)^* \;:\; S_x\mathscr{M} \to \mathcal{H}\,.$$

Multiplying e_x^ε by ι_x^ε gives us back the local correlation operator $F^\varepsilon(x)$. Namely,

$$\langle \psi \,|\, F^\varepsilon(x)\, \phi \rangle_{\mathcal{H}} = -\overline{(\mathfrak{R}_\varepsilon \psi)(x)} (\mathfrak{R}_\varepsilon \phi)(x) = -\overline{\left(e_x^\varepsilon \psi\right)} \left(e_x^\varepsilon \phi\right) = -\langle \psi \,|\, \iota_x^\varepsilon e_x^\varepsilon \phi \rangle_{\mathcal{H}}$$

and thus

$$F^\varepsilon(x) = -\iota_x^\varepsilon e_x^\varepsilon = -\iota_x^\varepsilon \left(\iota_x^\varepsilon\right)^* \;:\; \mathcal{H} \to \mathcal{H}\,. \tag{39}$$

The next proposition gives the desired connection between the spinor space $S_x\mathscr{M}$ and the corresponding spin space S_xM. We first state and prove the proposition and explain it afterwards.

Proposition 2.6 *The mapping*

$$e_x^\varepsilon|_{S_x} \;:\; S_xM \to S_x\mathscr{M} \quad \textit{is an isometric embedding}\,.$$

Moreover, under this embedding, the physical wave function of a vector u at x is mapped to the regularized Dirac wave function at x,

$$e_x^\varepsilon|_{S_x}\, \psi^u(x) = \big(\mathfrak{R}_\varepsilon u\big)(x)\,. \tag{40}$$

If the point x is regular (see Definition 1.5), the inverse is given by

$$\big(e_x^\varepsilon|_{S_x}\big)^{-1} = -\big(x|_{S_x}\big)^{-1} \iota_x^\varepsilon \;:\; S_x\mathscr{M} \to S_xM\,. \tag{41}$$

Proof Let $\psi, \phi \in S_xM$. Then

$$\overline{\big(e_x^\varepsilon \psi\big)}\big(e_x^\varepsilon \phi\big) = \langle \psi \,|\, (e_x^\varepsilon)^*\, e_x^\varepsilon\, \phi\rangle_{\mathcal{H}} = \langle \psi \,|\, \iota_x^\varepsilon\, e_x^\varepsilon\, \phi\rangle_{\mathcal{H}} \overset{(39)}{=} -\langle \psi \,|\, x\, \phi\rangle_{\mathcal{H}} = \prec\!\psi|\phi\!\succ .$$

Moreover, since the image of ι_x^ε coincides with S_xM, we know that e_x^ε vanishes on the orthogonal complement $S_x^\perp \subset \mathcal{H}$. Therefore,

$$e_x^\varepsilon|_{S_x}\, \psi^u(x) = e_x^\varepsilon|_{S_x}\, \pi_x\, u = e_x^\varepsilon\, u = \big(\mathfrak{R}_\varepsilon u\big)(x)\,.$$

Finally, if x is regular,

$$-\big(x|_{S_x}\big)^{-1} \iota_x^\varepsilon\, e_x^\varepsilon|_{S_xM} \overset{(39)}{=} \big(x|_{S_x}\big)^{-1}\, x|_{S_x} = \mathbb{1}_{S_x}\,,$$

proving that the inverse of $e_x^\varepsilon|_{S_x}$ is indeed given by the expression in (41). □

This proposition makes it possible to identify the spin space $S_xM \subset \mathcal{H}$ endowed with the inner product $\prec .|.\succ_x$ with a subspace of the spinor space $S_x\mathscr{M}$ with the inner product $\overline{\psi}\phi$. If the point x is singular, this is all we can expect, because in this case the spaces S_xM and $S_x\mathscr{M}$ have different dimensions and are clearly not isomorphic. As already mentioned after Definition 1.5, in most situations of physical interest the point x will be regular. In this case, we even obtain an isomorphism of S_xM and $S_x\mathscr{M}$ which preserves the inner products on these spaces. The identity (40) shows that, under the above identifications, the physical wave function ψ^u (as defined by (16)) goes over to the regularized Dirac wave function $(\mathfrak{R}_\varepsilon u)(x)$. This shows again that the causal fermion system involves the *regularized* objects. Moreover, one sees that the abstract formalism introduced in Sect. 1 indeed gives agreement with the usual objects in Minkowski space. We remark that the above isomorphism of S_xM and $S_x\mathscr{M}$ also makes it possible to use unambiguously the same notation for the corresponding inner product. Indeed, it is convenient denote the inner product on the Dirac spinors at a time point $x \in \mathscr{M}$ by

$$\prec .|.\succ_x \;:\; S_x\mathscr{M} \times S_x\mathscr{M} \to \mathbb{C}\,, \qquad \prec\!\psi|\phi\!\succ_x = \overline{\psi}\phi\,.$$

In order to avoid confusion, we avoided this notation so far. But from now on we will sometimes use it.

In the next proposition we compute the kernel of the fermionic projector $P^\varepsilon(x,y)$ (as defined by (11), where the subscript ε clarifies the dependence on the UV regularization) in Minkowski space. Moreover, we prove that the limit $\varepsilon \searrow 0$ exists in the distributional sense.

Proposition 2.7 *Assume that the points x and y are regular. Then, under the above identification of S_xM with $S_x\mathscr{M}$, the kernel of the fermionic projector has the representation*

$$P^\varepsilon(x,y) = -e_x^\varepsilon\, \iota_y^\varepsilon \;:\; S_y\mathscr{M} \to S_x\mathscr{M}\,.$$

Moreover, choosing an orthonormal basis (u_ℓ) of $\mathcal{H}$, the kernel of the fermionic projector can be written as

$$P^\varepsilon(x,y) = -\sum_\ell \big(\mathfrak{R}_\varepsilon u_\ell\big)(x)\, \overline{\big(\mathfrak{R}_\varepsilon u_\ell\big)(y)}\,. \tag{42}$$

In the limit $\varepsilon \searrow 0$, the kernel of the fermionic projector $P^\varepsilon(x,y)$ converges as a bi-distribution to the unregularized kernel defined by

$$P(x,y) := -\sum_\ell u_\ell(x)\, \overline{u_\ell(y)}\,. \tag{43}$$

More precisely, for every compact subset $K \subset \mathscr{M}$ and every $\delta > 0$, there is a constant $\varepsilon_0 > 0$ such that for all $\varepsilon \in (0,\varepsilon_0)$ and for all test wave functions $\eta, \tilde\eta \in C_0^\infty(K, S\mathscr{M})$,

$$\left| \iint_{\mathscr{M}\times\mathscr{M}} \overline{\eta(x)}\, \big(P^\varepsilon(x,y) - P(x,y)\big)\, \tilde\eta(y)\, d^4x\, d^4y \right| \leq \delta\, |\eta|_{C^1(K)}\, |\tilde\eta|_{C^1(K)}\,. \tag{44}$$

We remark that, since $\mathcal{H}$ is separable, we can always choose an at most countable orthonormal basis (u_ℓ) of $\mathcal{H}$.

Proof of Proposition 2.7 We first note that

$$P^\varepsilon(x,y) = e_x^\varepsilon\, \pi_x\, y\, \big(e_y^\varepsilon|_{S_y}\big)^{-1} = -e_x^\varepsilon\, \pi_x\, y\, \big(y|_{S_y}\big)^{-1}\, \iota_y^\varepsilon = -e_x^\varepsilon\, \pi_x\, \iota_y^\varepsilon = -e_x^\varepsilon\, \iota_y^\varepsilon\,.$$

In an orthonormal basis $(u)_\ell$, the completeness relation yields for any spinor $\chi \in S_y\mathscr{M}$

$$P^\varepsilon(x,y)\, \chi = -e_x^\varepsilon\, \iota_y^\varepsilon\, \chi = -\sum_\ell \big(e_x^\varepsilon\, u_\ell\big) \langle u_\ell \,|\, \iota_y^\varepsilon\, \chi\rangle_{\mathcal{H}} = -\sum_\ell \big(e_x^\varepsilon\, u_\ell\big)\, \big(\overline{e_x^\varepsilon\, u_\ell}\, \chi\big)\,,$$

and using (38) gives (42).

In order to prove (44), we introduce the functionals

$$\Phi^\varepsilon_\eta \;:\; \mathcal{H} \to \mathbb{C}\,, \qquad \Phi^\varepsilon_\eta u = \int_{\mathscr{M}} \overline{\eta(x)} \big(\mathfrak{R}_\varepsilon u\big)(x)\, d^4x$$

and similarly without UV regularization,

$$\Phi_\eta \;:\; \mathcal{H} \to \mathbb{C}\,, \qquad \Phi_\eta u = \int_{\mathscr{M}} \overline{\eta(x)}\, u(x)\, d^4x\,.$$

Then the left side of (44) can be written in the compact form

$$\big| \Phi^\varepsilon_\eta \left(\Phi^\varepsilon_{\tilde\eta}\right)^* - \Phi_\eta \left(\Phi_{\tilde\eta}\right)^* \big|\,,$$

which can be estimated with the triangle inequality by

$$\big| \Phi^\varepsilon_\eta \left(\Phi^\varepsilon_{\tilde\eta}\right)^* - \Phi_\eta \left(\Phi_{\tilde\eta}\right)^* \big| \leq \|\Phi^\varepsilon_\eta\| \,\big\|\Phi^\varepsilon_{\tilde\eta} - \Phi_{\tilde\eta}\big\| + \big\|\Phi^\varepsilon_\eta - \Phi_\eta\big\|\, \|\Phi_{\tilde\eta}\|\,. \tag{45}$$

It remains to estimate the operator norms in (45). To this end, we use property (iii) of Definition 2.3 in the following way: First, the norm of Φ_η can be estimated by

$$\big|\Phi_\eta u\big| = \int_{\mathscr{M}} \overline{\eta(x)}\, u(x)\, d^4x \leq |\eta|_{C^0(K)} \sqrt{\mu(K)} \left(\int_K |u(x)|\, d^4x \right)^{\frac{1}{2}},$$

and again by applying (33). This gives

$$\|\Phi_\eta\| \leq c\, |\eta|_{C^0(K)}\,.$$

Next, we use the triangle inequality together with (32) to obtain the inequality

$$\big\|\Phi^\varepsilon_\eta\big\| \leq \big\|\Phi^\varepsilon_\eta - \Phi_\eta\big\| \leq \delta\, |\eta|_{C^1(K)} + c\, |\eta|_{C^0(K)} \leq 2c\, |\eta|_{C^1(K)}\,,$$

valid uniformly for all $\varepsilon \in (0, \varepsilon_0)$ (note that property (i) cannot be used to obtain such a uniform estimate because we have no control on how the constant c in (30) depends on ε). Finally, again applying (32), we also know that

$$\big\|\Phi^\varepsilon_\eta - \Phi_\eta\big\| \leq \delta\, |\eta|_{C^1(K)}\,.$$

Using these inequalities in (45) gives the result. □

2.5 Correspondence of the Causal Structure

We now explain how the causal structure of Minkowski space is related to corresponding notions of a causal fermion system (see Definition 1.2 and the time direction (10)). To this end, we need to specify $\mathcal{H}$ as a closed subspace of the solution space of the vacuum Dirac equation (25). Clearly, this Dirac equation can be solved by the plane-wave ansatz

$$\psi(x) = e^{-ikx}\, \chi_k$$

with a constant spinor χ_k. Evaluating the resulting algebraic equation for χ shows that the momentum k must lie on the mass shell $k^2 = m^2$. The solutions on the upper and lower mass shell are the solutions of positive respectively negative energy. In order to avoid potential confusion with other notions of energy (like energy densities or energy expectation values), we here prefer the notion of solutions of positive and negative *frequency*. Taking Dirac's original concept literally, we here describe the vacuum in Minkowski space by the completely filled Dirac sea. Thus we choose $\mathcal{H}$ as the subspace of the solution space spanned by all plane-wave solutions of negative frequency. We refer to this choice as a *Dirac sea configuration*.

Lemma 2.8 *If $\mathcal{H}$ is the subspace of the solution space of the Dirac equation (25) spanned by all negative-frequency solutions, then the unregularized kernel of the fermionic projector as defined by (43) is the tempered bi-distribution*

$$P(x,y) = \int \frac{d^4k}{(2\pi)^4}\, (\not{k} + m)\, \delta(k^2 - m^2)\, \Theta(-k_0)\, e^{-ik(x-y)}\,, \tag{46}$$

where Θ is the Heaviside function, and $k(x-y)$ is a short notation for the Minkowski inner product $k_j\,(x-y)^j$.

Proof The integrand in (46) clearly is a tempered distribution. Hence its Fourier transform $P(x,y)$ is also a tempered distribution (in the vector $y-x$ and also in both vectors x and y). In addition, one verifies by direct computation that $P(x,y)$ is a distributional solution of the Dirac equation,

$$\begin{aligned}(i\partial\!\!\!/_x - m)\, P(x,y) &= \int \frac{d^4k}{(2\pi)^4}\, (\not{k} - m)(\not{k} + m)\, \delta(k^2 - m^2)\, \Theta(-k_0)\, e^{-ik(x-y)} \\ &= \int \frac{d^4k}{(2\pi)^4}\, \left(k^2 - m^2\right) \delta(k^2 - m^2)\, \Theta(-k_0)\, e^{-ik(x-y)} = 0\,.\end{aligned}$$

Due to the factor $\Theta(-k_0)$, the distribution $P(x,y)$ is composed of solutions of negative frequency. Moreover, since the matrix $(\not{k} + m)$ has rank two, one sees that $P(x,y)$ is indeed composed of *all* negative-frequency solutions. It remains to

show that the normalization of $P(x,y)$ is compatible with (43), meaning that

$$-2\pi \int_{\mathbb{R}^3} P\big(x,(t,\vec{y})\big)\, \gamma^0\, P\big((t,\vec{y}),z\big)\, d^3y = P(x,z)\,.$$

This identity follows by a straightforward computation: First,

$$\begin{aligned}
&\int_{\mathbb{R}^3} P\big(x,(t,\vec{y})\big)\, \gamma^0\, P\big((t,\vec{y}),z\big)\, d^3y \\
&\quad= \int_{\mathbb{R}^3} d^3y \int \frac{d^4k}{(2\pi)^4}\, e^{-ik(x-y)} \int \frac{d^4q}{(2\pi)^4}\, e^{-iq(y-z)}\, P_m(k)\, \gamma^0\, P_m(q) \qquad (47)\\
&\quad= \int \frac{d^4k}{(2\pi)^4} \int_{\mathbb{R}} \frac{d\lambda}{2\pi}\, e^{-ikx+iqz}\, P_m(k)\, \gamma^0\, P_m(q)\Big|_{q=(\lambda,\vec{k})}\,.
\end{aligned}$$

Setting $k=(\omega,\vec{k})$, we evaluate the δ-distributions inside the factors P_m,

$$\begin{aligned}
\delta(k^2-m^2)\,\delta(q^2-m^2)\big|_{q=(\lambda,\vec{k})} &= \delta\big(\omega^2-|\vec{k}|^2-m^2\big)\,\delta\big(\lambda^2-|\vec{k}|^2-m^2\big)\\
&= \delta(\lambda^2-\omega^2)\,\delta\big(\omega^2-|\vec{k}|^2-m^2\big)\,.
\end{aligned}$$

This shows that we only get a contribution if $\lambda = \pm\omega$. Using this fact together with the mass shell property $\omega^2-|\vec{k}|^2=m^2$, we can simplify the Dirac matrices according to

$$\begin{aligned}
(\not{k}+m)\,\gamma^0\,(\not{q}+m) &= (\omega\gamma^0+\vec{k}\vec{\gamma}+m)\,\gamma^0\,(\pm\omega\gamma^0+\vec{k}\vec{\gamma}+m)\\
&= (\omega\gamma^0+\vec{k}\vec{\gamma}+m)\,(\pm\omega\gamma^0-\vec{k}\vec{\gamma}+m)\,\gamma^0\\
&= \Big((\pm\omega^2+|\vec{k}|^2+m^2)\,\gamma^0 + (1\pm1)\,\omega\,(\vec{k}\vec{\gamma}) + (1\pm1)\,m\omega\Big)\\
&= \begin{cases} 2\omega\,(\not{k}+m) & \text{in case } +\\ 0 & \text{in case } -\,. \end{cases}
\end{aligned}$$

Hence we only get a contribution if $\lambda=\omega$, giving rise to the identity

$$\delta(\lambda^2-\omega^2) = \frac{1}{2|\omega|}\,\delta(\lambda-\omega)\,.$$

Putting these formulas together, we obtain

$$\int_{\mathbb{R}^3} P\big(x,(t,\vec{y})\big)\, \gamma^0\, P\big((t,\vec{y}),z\big)\, d^3y$$

$$= \int \frac{d^4k}{(2\pi)^4} \int_{\mathbb{R}} \frac{d\lambda}{2\pi}\, e^{-ik(x-z)}\, \delta(\lambda-\omega)\, \delta(k^2-m^2)\, \frac{2\omega}{2|\omega|}\, (\not{k}+m)\, \Theta(-k_0)$$
$$= -\frac{1}{2\pi} \int \frac{d^4k}{(2\pi)^4}\, e^{-ik(x-z)}\, \delta(k^2-m^2)\, (\not{k}+m)\, \Theta(-k_0)\,.$$

This gives the result. □

The Fourier integral (46) can be computed in closed form, giving an expression involving Bessel functions. In preparation, it is useful to pull the Dirac matrices out of the Fourier integral. To this end, one rewrites the factor $(\not{k}+m)$ in (46) in terms of a differential operator in position space,

$$P(x,y) = (i\partial\!\!\!/_x + m)\, T_{m^2}(x,y)\,, \tag{48}$$

where T_{m^2} is the scalar bi-distribution

$$T_{m^2}(x,y) := \int \frac{d^4k}{(2\pi)^4}\, \delta(k^2-m^2)\, \Theta(-k_0)\, e^{-ik(x-y)}\,.$$

In the next lemma, we determine the singular structure of this distribution. The method is to subtract an explicit singular distribution and to show that the difference is a *regular distribution* (i.e. a locally integrable function, denoted by L^1_{loc}). The distribution PP/ξ^2, denoted by *principal value*, is defined by evaluating weakly with a test function $\eta \in C_0^\infty(\mathscr{M})$ and by removing the positive and negative parts of the pole in a symmetric way. There are different equivalent ways of writing the principal part, each of which could serve as a possible definition:

$$\int \frac{\text{PP}}{\xi^2}\, \eta(\xi)\, d^4\xi = \lim_{\varepsilon \searrow 0} \int \Theta\big(|\xi^2| - \varepsilon\big)\, \frac{1}{\xi^2}\, \eta(\xi)\, d^4\xi$$
$$= \lim_{\varepsilon \searrow 0} \frac{1}{2} \sum_{\pm} \int \frac{1}{\xi^2 \pm i\varepsilon}\, \eta(\xi)\, d^4\xi = \lim_{\varepsilon \searrow 0} \frac{1}{2} \sum_{\pm} \int \frac{1}{\xi^2 \pm i\varepsilon\xi^0}\, \eta(\xi)\, d^4\xi\,.$$

Lemma 2.9 *On the light cone, the bi-distribution T_{m^2} has the following singularity structure,*

$$T_{m^2}(x,y) + \frac{1}{8\pi^3} \left(\frac{\text{PP}}{\xi^2} + i\pi\, \delta(\xi^2)\, \epsilon(\xi^0) \right) \in L^1_{\text{loc}}(\mathscr{M} \times \mathscr{M})\,, \tag{49}$$

where we set $\xi := y - x$. Away from the light cone (i.e. for $\xi^2 \neq 0$), $T_{m^2}(x,y)$ is a smooth function given by

$$T_{m^2}(x,y) = \begin{cases} \dfrac{m}{16\pi^2} \dfrac{Y_1\big(m\sqrt{\xi^2}\big)}{\sqrt{\xi^2}} + \dfrac{im}{16\pi^2} \dfrac{J_1\big(m\sqrt{\xi^2}\big)}{\sqrt{\xi^2}}\, \epsilon(\xi^0) & \text{if } \xi \text{ is timelike} \\ \dfrac{m}{8\pi^3} \dfrac{K_1\big(m\sqrt{-\xi^2}\big)}{\sqrt{-\xi^2}} & \text{if } \xi \text{ is spacelike}, \end{cases} \tag{50}$$

where J_1, Y_1 and K_1 are Bessel functions.

Proof The Fourier integral is computed most conveniently by inserting a convergence-generating factor. Thus for any $\varepsilon > 0$ we consider the Fourier integral

$$T^\varepsilon_{m^2}(x,y) := \int \frac{d^4k}{(2\pi)^4}\, \delta(k^2 - m^2)\, \Theta(-k_0)\, e^{-ik(x-y)}\, e^{-\varepsilon\,|k_0|}\,.$$

This Fourier integral can be computed pointwise, showing that $T^\varepsilon(x,y)$ is a regular distribution. Taking the limit $\varepsilon \searrow 0$ in the distributional sense, we will then obtain $T_{m^2}(x,y)$.

Setting $\xi = y - x$ and $t = \xi^0$, we first carry out the integral over k_0 to obtain

$$\begin{aligned} T^\varepsilon_{m^2}(x,y) &= \int \frac{d^4k}{(2\pi)^4}\, \delta(k^2 - m^2)\, \Theta(-k_0)\, e^{ik\xi}\, e^{-\varepsilon\,|k_0|} \\ &= \int_{\mathbb{R}^3} \frac{d^3k}{(2\pi)^4}\, \frac{1}{2\sqrt{\vec{k}^2 + m^2}}\, e^{-i\sqrt{\vec{k}^2+m^2}\,t - i\vec{k}\vec{\xi}}\, e^{-\varepsilon\sqrt{\vec{k}^2+m^2}}\,. \end{aligned}$$

Next, for the spatial momentum $\vec{k}$ we introduce polar coordinates ($p = |\vec{k}|, \vartheta, \varphi$), where ϑ is the angle between $\vec{k}$ and $\vec{\xi}$, and φ is the azimuthal angle. Also setting $r = |\vec{\xi}|$, we get

$$\begin{aligned} T^\varepsilon_{m^2}(x,y) &= \int_0^\infty \frac{dp}{2(2\pi)^3} \int_{-1}^1 d\cos\theta\, \frac{p^2}{\sqrt{p^2+m^2}}\, e^{-(\varepsilon+it)\sqrt{p^2+m^2}}\, e^{-ipr\cos\theta} \\ &= \frac{1}{r} \int_0^\infty \frac{dp}{(2\pi)^3}\, \frac{p}{\sqrt{p^2+m^2}}\, e^{-(\varepsilon+it)\sqrt{p^2+m^2}}\, \sin(pr) \\ &= \frac{m^2}{(2\pi)^3} \frac{K_1\big(m\sqrt{r^2 + (\varepsilon+it)^2}\big)}{m\sqrt{r^2+(\varepsilon+it)^2}}, \end{aligned} \tag{51}$$

where the last integral was carried out using [29, formula (3.961.1)]. Here the square root and the Bessel function K_1 is defined as usual using a branch cut along the negative real axis.

When taking the limit $\varepsilon \searrow 0$, one must be careful for two reasons. First, a pole forms on the light cone $t = \pm r$. Second, the Bessel function K_1 involves logarithms, which must be evaluated in the complex plane using the branch cut along the negative real axis. For clarity, we treat these two issues after each other. The asymptotic expansion of the Bessel function (see [34, (10.31.1)])

$$K_1(z) = \frac{1}{z} + \mathcal{O}\big(z \log z\big)$$

yields that the pole on the light cone is of the form

$$T^\varepsilon_{m^2}(x,y) = \frac{1}{(2\pi)^3}\, \frac{1}{r^2 + (\varepsilon + it)^2} + \mathcal{O}\big(\log |\xi^2|\big)\,,$$

uniformly in ε. Therefore, after subtracting the pole, we can take the limit $\varepsilon \searrow 0$ as a locally integrable function, i.e.

$$\lim_{\varepsilon \searrow 0} \left(T^\varepsilon_{m^2}(x,y) - \frac{1}{(2\pi)^3}\, \frac{1}{r^2 + (\varepsilon + it)^2} \right) \in L^1_{\text{loc}}(\mathscr{M} \times \mathscr{M})\,.$$

For the subtracted pole, the limit $\varepsilon \searrow 0$ can be computed in the distributional sense by

$$\lim_{\varepsilon \searrow 0} \frac{1}{r^2 + (\varepsilon + it)^2} = \lim_{\varepsilon \searrow 0} \frac{1}{r^2 - t^2 + i\varepsilon t} = -\frac{\text{PP}}{\xi^2} - i\pi\, \delta(\xi^2)\, \epsilon(\xi^0)\,,$$

where we used the distributional equation

$$\lim_{\varepsilon \searrow 0} \left(\frac{1}{x - i\varepsilon} - \frac{1}{x + i\varepsilon} \right) = 2\pi i\, \delta(x)\,.$$

Here "PP" again denotes the principal value, and ϵ is the step function $\epsilon(x) = 1$ for $x \geq 0$ and $\epsilon(x) = -1$ otherwise. This gives (49).

In order to compute the regular part of the distribution T_{m^2}, we may disregard the singularity on the light cone and may consider the case that ξ is either spacelike or timelike. In the first case, the argument $m\sqrt{r^2 + (\varepsilon + it)^2}$ of the Bessel function converges to the positive real axis, where the Bessel function is analytic. This gives the lower equation in (50). In the remaining case that ξ is timelike, the argument $m\sqrt{r^2 + (\varepsilon + it)^2}$ converges to the imaginary axis (more precisely, to the upper imaginary axis if $t > 0$ and to the lower imaginary axis if $t < 0$). Using the relations [34, (10.27.9) and (10.27.10)]

$$i\pi J_1(z) = -iK_1(-iz) - iK_1(iz) \qquad \text{and} \qquad -\pi Y_1(z) = -iK_1(-iz) + iK_1(iz)$$

(valid if $|\arg z| < \frac{\pi}{2}$), one can express K_1 near the upper and lower imaginary axis by

$$K_1(\pm iz) = -\frac{\pi}{2}\big(J_1(z) \mp iY_1(z)\big)\,.$$

Using these identities in (51) and using that the Bessel functions J_1 and K_1 are analytic in a neighborhood of the positive real axis, one can take the limit $\varepsilon \searrow 0$ to obtain the upper equation in (50). □

We point out that the Bessel functions in (50) are all real-valued. In particular, one sees that $T(x,y)$ is real-valued if the vector ξ is spacelike.

Using the result of Lemma 2.9 in (48), one can derive corresponding formulas for $P(x,y)$. In particular, differentiating (49), one sees that $P(x,y)$ has an even stronger singularity on the light cone which involves terms of the form $1/\xi^4$ and $\delta'(\xi^2)$. Differentiating (50), carrying out the derivatives with the chain rule and using formulas for the derivatives of Bessel functions (see [34, (10.6.6) and (10.29.4)]), one can also express the fermionic projector $P(x,y)$ in terms of Bessel functions. We do not give the resulting formulas, because we do not need the detailed form later on. Instead, we here prefer to argue with general properties of the distribution $P(x,y)$. This makes it possible to infer qualitative properties of the eigenvalues of A_{xy}, even without referring to the detailed form of the formulas in Lemma 2.9. From Lorentz symmetry, we know that for all x and y with spacelike or timelike separation, $P(x,y)$ can be written as

$$P(x,y) = \alpha\, \xi_j \gamma^j + \beta\, \mathbb{1} \tag{52}$$

with two complex-valued functions α and β (where again $\xi = y - x$). Taking the conjugate with respect to the spin scalar product, we see that

$$P(y,x) = \overline{\alpha}\, \xi_j \gamma^j + \overline{\beta}\, \mathbb{1}\,. \tag{53}$$

As a consequence,

$$A_{xy} = P(x,y)\, P(y,x) = a\, \xi_j \gamma^j + b\, \mathbb{1} \tag{54}$$

with two real parameters a and b given by

$$a = \alpha\overline{\beta} + \beta\overline{\alpha}\,, \qquad b = |\alpha|^2\, \xi^2 + |\beta|^2\,. \tag{55}$$

Applying the formula $(A_{xy} - b\mathbb{1})^2 = a^2\, \xi^2\, \mathbb{1}$, the roots of the characteristic polynomial of A_{xy} are computed by

$$b \pm \sqrt{a^2\, \xi^2}\,. \tag{56}$$

Therefore, the eigenvalues of the closed chain are either real, or else they form a complex conjugate pair. Which of the two cases appears is determined by the sign of the factor ξ^2. This gives the agreement of the different notions of causality in the following sense:

Proposition 2.10 *Assume that $P(x,y)$ is the unregularized kernel of the fermionic projector of the vacuum (46), and that the eigenvalues $\lambda_1^{xy}, \ldots, \lambda_4^{xy}$ are computed as the eigenvalues of the closed chain (12). Then the following statements hold: If the points $x, y \in \mathscr{M}$ have spacelike separation in Minkowski space, then they are also spacelike separated in the sense of Definition 1.2. If, on the other hand, the points $x, y \in \mathscr{M}$ have timelike separation in Minkowski space, then they are also timelike separated in the sense of Definition 1.2. Even more, they are properly timelike separated (see Definition 1.6) in the sense that the closed chain A_{xy} has strictly positive eigenvalues and definite eigenspaces. Finally, if the points $x, y \in \mathscr{M}$ have lightlike separation in Minkowski space, then the causal structure of Definition 1.2 is ill-defined.*

The fact that the causal structure is ill-defined for lightlike separation again explains why an UV regularization must be introduced.

Proof of Proposition 2.10 If the vector $\xi = y - x$ is spacelike, then the term ξ^2 is negative. Thus the eigenvalues in (56) form a complex conjugate pair, implying that they all have the same absolute value. Thus the points are spacelike separated in the sense of Definition 1.2.

If the vector ξ is timelike, the term ξ^2 in (56) is positive, so that the λ_j are all real. In order to show that they do not have the same absolute value, we need to verify that the parameters a and b are both non-zero. This makes it necessary to refer to the explicit formula involving Bessel functions (50): The Bessel functions Y_1 and J_1 do not have joint zeros on the positive real axis. As a consequence, the parameter β in (52) is non-zero. Likewise, the derivatives Y_1' and J_1' do not have joint zeros (as can again be verified from the fact that the Bessel functions form a fundamental system). This implies that the parameter α in (52) is non-zero. We conclude that the parameter b in (55) is non-zero. The combination of α and β in the formula for a in (55) can be rewritten in terms of a Wronskian of the Bessel function. This Wronskian can be computed explicitly using [34, (10.5.2)], implying that a is non-zero. We conclude that the points x and y are timelike separated in the sense of Definition 1.2.

In order to get the connection to proper timelike separation, recall that if ξ is a timelike vector of Minkowski space, then the closed chain has the form (55) with $a, b \neq 0$. A direct computation shows that this matrix is diagonalizable and that the eigenspaces are definite with respect to the spin scalar product. Moreover, applying the Schwarz inequality to the explicit formulas (55), one obtains

$$|a|\sqrt{\xi^2} = 2\,\mathrm{Re}\left(\alpha\sqrt{\xi^2}\,\overline{\beta}\right) \overset{(\star)}{\leq} |\alpha|^2\xi^2 + |\beta|^2 = b\,, \tag{57}$$

proving that the eigenvalues in (56) are non-negative. It remains to show that none of these eigenvalues vanishes. To this end, it suffices to show that the inequality ($\star$) in (57) is strict, which in turn is equivalent to proving that

$$\mathrm{Im}\left(\alpha\overline{\beta}\right) \neq 0\,.$$

This inequality follows by a detailed analysis of the Bessel functions (see [14, proof of Lemma 4.3]). We conclude that x and y are indeed properly timelike separated.

If the vector ξ is lightlike, then $P(x,y)$ is not defined pointwise. As a consequence, the closed chain is ill-defined. □

This proposition cannot be applied directly to causal fermion systems because, as explained in Sects. 2.1 and 2.2, constructing a causal fermion system makes it necessary to introduce an UV regularization. Nevertheless, the above proposition also gives correspondence of the different notions of causality for causal fermion systems describing the Minkowski vacuum, as we now explain. Thus let us consider the causal fermion system corresponding to the regularized fermionic projector of the vacuum $P^\varepsilon(x,y)$. In the limit $\varepsilon \searrow 0$, the kernel of the fermionic projector $P^\varepsilon(x,y)$ converges to the unregularized kernel $P(x,y)$ (see (44) in Proposition 2.6). If this convergence is pointwise, i.e. if for given space-time points $x, y \in \mathscr{M}$,

$$\lim_{\varepsilon \searrow 0} P^\varepsilon(x,y) = P(x,y)\,, \tag{58}$$

then the results of Proposition 2.10 also apply to the causal fermion system, up to error terms which tend to zero as $\varepsilon \searrow 0$. Thinking of ε as the Planck scale, this means physically that the notion of causality of Definition 1.2 agrees with the usual notion of causality in Minkowski space, up to corrections which are so small that they cannot be observed. The subtle point of this argument is that it requires pointwise convergence (58). Clearly, such a pointwise convergence cannot hold if x and y are lightlike separated, because the right side of (58) is ill-defined pointwise. Expressed for a causal fermion system for fixed ε on the Planck scale, this means that the notion of causality of Definition 1.2 does *not* agree with the usual notion of causality if the vector ξ is almost lightlike in the sense that $\big||\xi^0| - |\vec{\xi}|\big| \lesssim \varepsilon$. This is not surprising because we cannot expect that the notion of causality in Minkowski space holds with a higher resolution than the regularization scale ε. The remaining question is whether we have pointwise convergence (58) if the points x and y have timelike or spacelike separation. The answer is yes for a large class of regularizations (like for example the regularization by mollification in Example 2.4). However, the general notion of Definition 2.3 only gives weak convergence of the kernels (44). This shortcoming could be removed by adding a condition to Definition 2.3 which ensures pointwise convergence away from the light cone. On the other hand, such an additional condition seems unnecessary, and therefore it seems preferable not to impose it. Nevertheless, the physical picture is that the regularized kernel should converge pointwise, at least for generic points x and y which lie sufficiently far away from the light cone. With this in

mind, Proposition 2.10 indeed shows that the notion of causality of Definition 1.2 corresponds to the usual notion of causality in Minkowski space, up to corrections which are so small that they are irrelevant in most situations of interest.

We conclude this section by explaining why the functional $\mathcal{C}$ introduced in (9) gives information on the time direction. Our first task is to rewrite this functional in terms of the regularized kernel of the fermionic projector $P^\varepsilon(x,y)$.

Lemma 2.11 *Assume that the operator $P^\varepsilon(x,x) : S_x\mathscr{M} \to S_x\mathscr{M}$ is invertible. Then, setting*

$$\nu(x) = P^\varepsilon(x,x)^{-1} \;:\; S_x\mathscr{M} \to S_x\mathscr{M}\,, \tag{59}$$

the functional $\mathcal{C}$, (9), can be written as

$$\mathcal{C}(x,y) = i\,\mathrm{Tr}_{S_x}\Big(P^\varepsilon(x,y)\,\nu(y)\,P^\varepsilon(y,x)\,\big[\nu(x), A_{xy}\big]\Big)\,. \tag{60}$$

Proof Since $P(x,x) = \pi_x x|_{S_x} = x|_{S_x}$, we know that $\nu(x) = (x|_{S_x})^{-1}$. Thus

$$\begin{aligned}\pi_x\, y\, x\, \pi_y\, \pi_x|_{S_x} &= \pi_x y\, \pi_y x\, \pi_x y\, \nu(y)\, \pi_y x\, \nu(x)|_{S_x} \\ &= P^\varepsilon(x,y)\,P^\varepsilon(y,x)\,P^\varepsilon(x,y)\,\nu(y)\,P^\varepsilon(y,x)\,\nu(x)|_{S_x}\,.\end{aligned}$$

Using this formula in (9), we obtain

$$\begin{aligned}\mathcal{C}(x,y) &= i\,\mathrm{Tr}_{S_x}\big(y\,x\,\pi_y\,\pi_x|_{S_x} - y\,\pi_x\,\pi_y\,x|_{S_x}\big) \\ &= i\,\mathrm{Tr}_{S_x}\Big(P^\varepsilon(x,y)\,P^\varepsilon(y,x)\,P^\varepsilon(x,y)\,\nu(y)\,P^\varepsilon(y,x)\,\nu(x) \\ &\qquad - P^\varepsilon(x,y)\,P^\varepsilon(y,x)\,\nu(x)\,P^\varepsilon(x,y)\,\nu(y)\,P^\varepsilon(y,x)\Big) \\ &= i\,\mathrm{Tr}_{S_x}\Big(P^\varepsilon(x,y)\,\nu(y)\,P^\varepsilon(y,x)\,\nu(x)\,P^\varepsilon(x,y)\,P^\varepsilon(y,x) \\ &\qquad - P^\varepsilon(x,y)\,\nu(y)\,P^\varepsilon(y,x)\,P^\varepsilon(x,y)\,P^\varepsilon(y,x)\,\nu(x)\Big)\,.\end{aligned}$$

This gives the result. □

We point out that the operator $\nu(x)$ in (59) is ill-defined without UV regularization because evaluating the distribution $P(x,y)$ on the diagonal $x = y$ has no mathematical meaning. As a consequence, the functional $\mathcal{C}$ is ill-defined without UV regularization, even if x and y have timelike separation. This makes the following computation somewhat delicate. In order to keep the analysis reasonably simple, we assume that the regularized kernel of the fermionic projector has *vector-scalar structure*, meaning that it is of the general form

$$P^\varepsilon(x,y) = v_j^\varepsilon(x,y)\,\gamma^j \;+\; \beta^\varepsilon(x,y)\,\mathbb{1} \tag{61}$$

with a vectorial and a scalar component. Here $v^\varepsilon(x,y)$ is a complex vector field (i.e. it can be written as $v^\varepsilon = u^\varepsilon + iw^\varepsilon$ with Minkowski vectors u^ε and w^ε which need not be collinear). Then, evaluating (61) for $x = y$, one sees that $P^\varepsilon(x,x)$ can be written as

$$P^\varepsilon(x,x) = v_j^\varepsilon(x)\, \gamma^j \;+\; \beta^\varepsilon(x)\, \mathbb{1}$$

(where we set $v^\varepsilon(x) = v^\varepsilon(x,x)$ and $\beta^\varepsilon(x) = \beta^\varepsilon(x,x)$). Since $P^\varepsilon(x,x)$ is a symmetric operator on $S_x\mathscr{M}$, it follows that v^ε is a real vector field, and β a real-valued function. For a large class of regularizations, the matrix $P^\varepsilon(x,x)$ is invertible because the vectorial component dominates the scalar component. With this in mind, we here assume that $\nu(x)$ exists. Then it is given by

$$\nu(x) = \frac{1}{\rho(x)} \left(v_j^\varepsilon(x)\, \gamma^j - \beta^\varepsilon(x)\, \mathbb{1} \right), \tag{62}$$

where $\rho := v_j^\varepsilon (v^\varepsilon)^j - (\beta^\varepsilon)^2$. Now we can compute the composite expression in (60), working for all other terms with the unregularized formulas (which is again justified if we have pointwise convergence (58)). This gives the following result.

Proposition 2.12 *Using (62) and replacing $P^\varepsilon(x,y)$, $P^\varepsilon(y,x)$ and A_{xy} by the unregularized expressions (52), (53) and (54), the functional $\mathcal{C}$ is given by*

$$\mathcal{C}(x,y) = \frac{16a}{\rho(x)\,\rho(y)}\, \mathrm{Im}\left(\alpha\overline{\beta}\right) \left(v^\varepsilon(x)^j\, \xi_j\, v^\varepsilon(y)^k\, \xi_k - \xi^2\, v^\varepsilon(x)^j\, v^\varepsilon(y)_j \right). \tag{63}$$

Proof Using (62) and (54) in (60) gives

$$\begin{aligned} \mathcal{C}(x,y) &= i\,\mathrm{Tr}_{S_x}\Big(P(x,y)\, \nu(y)\, P(y,x) \left[\nu(x), A_{xy} \right] \Big) \\ &= \frac{ia}{\rho(x)}\, \mathrm{Tr}_{S_x}\Big(P(x,y)\, \nu(y)\, P(y,x) \left[\not{v}^\varepsilon(x), \not{\xi} \right] \Big), \end{aligned}$$

where in the last step we used that the scalar components of A_{xy} and $\nu(x)$ drop out of the commutator. Taking the scalar component of $\nu(y)$, the two factors $P(x,y)$ and $P(y,x)$ combine to the closed chain, which according to (54) has no bilinear component, so that the trace vanishes. Therefore, we only need to take into account the vectorial component of $\nu(y)$. Using (52) and (53), we obtain

$$\begin{aligned} \mathcal{C}(x,y) &= \frac{ia}{\rho(x)\,\rho(y)}\, \mathrm{Tr}_{S_x}\Big(\left(\alpha \not{\xi} + \beta\, \mathbb{1}\right) \not{v}^\varepsilon(y) \left(\overline{\alpha} \not{\xi} + \overline{\beta}\, \mathbb{1}\right) \left[\not{v}^\varepsilon(x), \not{\xi} \right] \Big) \\ &= -\frac{a}{\rho(x)\,\rho(y)}\, \mathrm{Im}\left(\alpha\overline{\beta}\right)\, \mathrm{Tr}_{S_x}\Big(\left[\not{\xi}, \not{v}^\varepsilon(y) \right] \left[\not{v}^\varepsilon(x), \not{\xi} \right] \Big). \end{aligned}$$

Computing the trace of the product of Dirac matrices gives the result. □

For the interpretation of the formula (63), we first consider the case that y and x have space-like separation. In this case, it turns out that the prefactor $\mathrm{Im}(\alpha\overline{\beta})$ vanishes, so that (63) gives no information on a time direction. This is consistent with the fact that for points in Minkowski space with space-like separation, the notions of future- and past-directed depend on the observer and cannot be defined in a covariant manner. However, if y and x have timelike separation, then the factors a and $\mathrm{Im}(\alpha\overline{\beta})$ are indeed both non-zero (see the proof of Proposition 2.10). Therefore, the functional $\mathcal{C}$ is non-zero, provided that the vector ξ is *non-degenerate* in the sense that it is linearly independent of both $v^\varepsilon(x)$ and $v^\varepsilon(y)$. Since the set of directions ξ for which these vectors are linearly dependent has measure zero, we may always restrict attention to non-degenerate directions. Moreover, the formula (63) shows that the functional $\mathcal{C}$ does not change sign for ξ inside the upper or lower light cone. On the other hand, $\mathcal{C}$ is antisymmetric under sign flips of ξ because interchanging x and y in (9) obviously gives a minus sign.

We conclude that for the regularized Dirac sea vacuum, the sign of the functional $\mathcal{C}$ distinguishes a time direction. Asymptotically as $\varepsilon \searrow 0$, this time direction agrees with the distinction of the causal past and causal future in Minkowski space.

To summarize, in this section we saw how the intrinsic structures of a causal fermion system correspond to the usual structures in Minkowski space. To this end, we constructed causal fermion systems from a regularized Dirac sea configuration and analyzed the asymptotics as the UV regularization is removed. For brevity, we only considered the topological and causal structure of space-time as well as spinors and wave functions. The reader interested in geometric structures like connection and curvature is referred to the detailed exposition in [14]. Moreover, in Sect. 5 below we shall explain how the methods and results introduced in this section can be generalized to interacting systems.

3 Underlying Physical Principles

In order to clarify the physical concepts, we now briefly discuss the underlying physical principles. Causal fermion systems evolved from an attempt to combine several physical principles in a coherent mathematical framework. As a result, these principles appear in the framework in a specific way:

- The **principle of causality** is built into a causal fermion system in a specific way, as was explained in Sect. 1.2 above.
- The **Pauli exclusion principle** is incorporated in a causal fermion system, as can be seen in various ways. One formulation of the Pauli exclusion principle states that every fermionic one-particle state can be occupied by at most one particle. In this formulation, the Pauli exclusion principle is respected because every wave function can either be represented in the form ψ^u (the state is occupied) with $u \in \mathcal{H}$ or it cannot be represented as a physical wave function (the state is not occupied). Via these two conditions, the fermionic projector encodes for every state the occupation numbers 1 and 0, respectively, but it is impossible

to describe higher occupation numbers. More technically, one may obtain the connection to the fermionic Fock space formalism by choosing an orthonormal basis $u_1, \ldots, u_f$ of $\mathcal{H}$ and forming the f-particle Hartree-Fock state

$$\Psi := \psi^{u_1} \wedge \cdots \wedge \psi^{u_f} .$$

Clearly, the choice of the orthonormal basis is unique only up to the unitary transformations

$$u_i \to \tilde{u}_i = \sum_{j=1}^{f} U_{ij}\, u_j \quad \text{with} \quad U \in \mathrm{U}(f) .$$

Due to the anti-symmetrization, this transformation changes the corresponding Hartree-Fock state only by an irrelevant phase factor,

$$\psi^{\tilde{u}_1} \wedge \cdots \wedge \psi^{\tilde{u}_f} = \det U\; \psi^{u_1} \wedge \cdots \wedge \psi^{u_f} .$$

Thus the configuration of the physical wave functions can be described by a fermionic multi-particle wave function. The Pauli exclusion principle becomes apparent in the total anti-symmetrization of this wave function.

► A **local gauge principle** becomes apparent once we choose basis representations of the spin spaces and write the wave functions in components. Denoting the signature of $(S_x, \prec.|.\succ_x)$ by $(p(x), q(x))$, we choose a pseudo-orthonormal basis $(\mathfrak{e}_\alpha(x))_{\alpha=1,\ldots,p+q}$ of S_x. Then a wave function ψ can be represented as

$$\psi(x) = \sum_{\alpha=1}^{p+q} \psi^\alpha(x)\; \mathfrak{e}_\alpha(x)$$

with component functions $\psi^1, \ldots, \psi^{p+q}$. The freedom in choosing the basis $(\mathfrak{e}_\alpha)$ is described by the group $\mathrm{U}(p, q)$ of unitary transformations with respect to an inner product of signature (p, q). This gives rise to the transformations

$$\mathfrak{e}_\alpha(x) \to \sum_{\beta=1}^{p+q} U^{-1}(x)^\beta_\alpha\; \mathfrak{e}_\beta(x) \qquad \text{and} \qquad \psi^\alpha(x) \to \sum_{\beta=1}^{p+q} U(x)^\alpha_\beta\; \psi^\beta(x)$$

with $U \in \mathrm{U}(p, q)$. As the basis $(\mathfrak{e}_\alpha)$ can be chosen independently at each spacetime point, one obtains *local gauge transformations* of the wave functions, where the gauge group is determined to be the isometry group of the spin scalar product. The causal action is *gauge invariant* in the sense that it does not depend on the choice of spinor bases.

► The **equivalence principle** is incorporated in the following general way. Spacetime $M := \operatorname{supp} \rho$ together with the universal measure ρ form a topological measure space, being a more general structure than a Lorentzian manifold. Therefore, when describing M by local coordinates, the freedom in choosing

such coordinates generalizes the freedom in choosing general reference frames in a space-time manifold. Therefore, the equivalence principle of general relativity is respected. The causal action is *generally covariant* in the sense that it does not depend on the choice of coordinates.

4 The Dynamics of Causal Fermion Systems

Similar to the Einstein-Hilbert action in general relativity, in the causal action principle one varies space-time as well as all structures therein globally. This global viewpoint implies that it is not obvious what the causal action principle tells us about the dynamics of the system. The first step for clarifying the situation is to derive the Euler-Lagrange (EL) equations corresponding to the causal action principle (Sect. 4.1). Similar to the Einstein or Maxwell equations, these EL equations should describe the dynamics. Additional insight is gained by studying Noether-like theorems which specify the quantities which are conserved in the dynamics (Sect. 4.2). Finally, we review results on the initial value problem (Sect. 4.3). We remark that more explicit information on the dynamics is obtained by considering limiting cases in which the EL equations corresponding to the causal action reduce to equations of a structure familiar from classical field theory and quantum field theory (see Sect. 5).

4.1 The Euler-Lagrange Equations

We now return to the abstract setting of Sect. 1. Our goal is to derive the EL equations corresponding to the causal action principle in the form most useful for our purposes. The method is to consider so-called *variations of the physical wave functions* which we now introduce (for more general variations see Remark 4.3 below). Let $(\mathcal{H}, \mathcal{F}, \rho)$ be a causal fermion system. We assume that ρ is a minimizer of the causal action principle. However, we do not want to assume that the total volume $\rho(\mathcal{F})$ be finite. Instead, we merely assume that ρ is *locally finite* in the sense that $\rho(K) < \infty$ for every compact subset $K \subset \mathcal{F}$. Our starting point is the wave evaluation operator Ψ introduced in (18),

$$\Psi \;:\; \mathcal{H} \to C^0(M, SM)\,, \qquad u \mapsto \psi^u\,.$$

We now vary the wave evaluation operator. Thus for any $\tau \in (-\delta, \delta)$ we consider a mapping $\Psi_\tau : \mathcal{H} \to C^0(M)$. For $\tau = 0$, this mapping should coincide with the wave evaluation operator Ψ. The family $(\Psi_\tau)_{\tau \in (-\delta, \delta)}$ can be regarded as a simultaneous variation of all physical wave functions of the system. In fact, for any $u \in \mathcal{H}$, the variation of the corresponding physical wave function is given by

$$\psi^u_\tau := \Psi_\tau(u) \in C^0(M, SM)\,.$$

Next, we introduce the corresponding local correlation operators F_τ by

$$F_\tau(x) := -\Psi_\tau(x)^* \Psi_\tau(x) \qquad \text{so that} \qquad F_\tau : M \to \mathcal{F}\,.$$

In view of (19), we know that $F_0(x) = x$. Therefore, the family $(F_\tau)_{\tau \in (-\delta,\delta)}$ is a variation of the local correlation operators. Taking the push-forward measure gives rise to a family of universal measures,

$$\rho_\tau := (F_\tau)_* \rho\,. \tag{64}$$

Since F_0 is the identity, we know that $\rho_0 = \rho$. Therefore, the family $(\rho_\tau)_{\tau \in (-\delta,\delta)}$ is indeed a variation of the universal measure.

We now work out the EL equations for the resulting class of variations of the universal measure. In order for the constructions to be mathematically well-defined, we need a few technical assumptions which are summarized in the following definition.

Definition 4.1 The **variation of the physical wave functions** is **smooth** and **compact** if the family of operators $(\Psi_\tau)_{\tau \in (-\delta,\delta)}$ has the following properties:

(a) The variation is trivial on the orthogonal complement of a finite-dimensional subspace $I \subset \mathcal{H}$, i.e.

$$\Psi_\tau|_{I^\perp} = \Psi \qquad \text{for all } \tau \in (-\delta, \delta)\,.$$

(b) There is a compact subset $K \subset M$ outside which the variation is trivial, i.e.

$$\big(\Psi_\tau(u)\big)\big|_{M \setminus K} = \big(\Psi(u)\big)\big|_{M \setminus K} \qquad \text{for all } \tau \in (-\delta, \delta) \text{ and } u \in \mathcal{H}\,.$$

(c) The Lagrangian is continuously differentiable in the sense that the derivative

$$\frac{d}{d\tau} \mathcal{L}\big(x, F_\tau(y)\big)\big|_{\tau=0} \tag{65}$$

exists and is continuous on $M \times M$.

With the conditions (a) and (b) we restrict attention to variations which are sufficiently well-behaved (similar as in the classical calculus of variations, where one restricts attention to smooth and compactly supported variations). It is a delicate point to satisfy the condition (c), because (due to the absolute values of the eigenvalues in (1)) the Lagrangian is only Lipschitz continuous on $\mathcal{F} \times \mathcal{F}$. Therefore, the derivative in (65) does not need to exist, even if $F_\tau(y)$ is smooth. This means that in the applications, one must verify that the condition (c) holds (for details see the computations in [6]). Here we simply assume that the variation of the wave functions is smooth and compact.

By definition of the push-forward measure (64), we know that for any integrable function f on $\mathcal{F}$,

$$\int_{\mathcal{F}} f(x)\, d\rho_\tau = \int_{\mathcal{F}} f(F_\tau(x))\, d\rho\,. \tag{66}$$

In this way, the variation of the measure can be rewritten as a variation of the arguments of the integrand. In particular, the variation of the action can be written as

$$\iint_{M\times M} \mathcal{L}\big(F_\tau(x), F_\tau(y)\big)\, d\rho(x)\, d\rho(y)$$

(and similarly for the other integrals). Another benefit of working with the push-forward measure (64) is that the total volume is preserved. Namely, combining the identity (66) with the assumption in Definition 4.1(b), one readily verifies that the volume constraint (3) is satisfied in the sense that ρ_τ satisfies the conditions (7).

We consider first variations, treating the constraints with Lagrange multipliers (this procedure is justified in [1]). Since the volume constraint is already respected, it remains to consider the trace constraint (4) and the boundedness constraint (5). We conclude that first variations of the functional

$$\mathcal{S}_{\kappa,\lambda} := \mathcal{S} + \kappa\,\big(\mathcal{T} - C\big) - \lambda\left(\int_{\mathcal{F}} \mathrm{tr}(x)\, d\rho - c\right) \tag{67}$$

vanish for suitable values of the Lagrange parameters $\kappa, \lambda \in \mathbb{R}$, where the constants C and c are the prescribed values of the constraints. For clarity, we point out that the boundedness constraint merely is an inequality. The method for handling this inequality constraint is to choose $\kappa = 0$ if $\mathcal{T}(\rho) < C$, whereas in the case $\mathcal{T}(\rho) = C$ the Lagrange multiplier κ is in general non-zero (for details see again [1]). Introducing the short notation

$$\mathcal{L}_\kappa(x,y) := \mathcal{L}(x,y) + \kappa\,|xy|^2\,,$$

we can write the effective action as

$$\mathcal{S}_{\kappa,\lambda}(\rho_\tau) = \iint_{M\times M} \mathcal{L}_\kappa(x,y)\, d\rho(x)\, d\rho(y) - \lambda \int_M \mathrm{tr}\big(F_\tau(x)\big)\, d\rho(x) - \kappa C + \lambda c\,.$$

Now we can compute the first variation by differentiating with respect to τ. It is most convenient to express the causal action and the constraints in terms of the kernel of the fermionic projector (just as explained at the beginning of Sect. 1.3). Moreover, it is preferable to consider the Lagrangian $\mathcal{L}_\kappa(x,y)$ as a function only of $P_\tau(x,y)$ by writing the closed chain as

$$A_{xy} = P_\tau(x,y)\, P_\tau(x,y)^* \tag{68}$$

(where $P_\tau(x,y)^*$ denotes similar to (13) the adjoint with respect to the spin scalar product). We use the notation

$$\delta P(x,y) = \frac{d}{d\tau} P_\tau(x,y)\Big|_{\tau=0},$$

and similarly for other functions. When computing the variation of the Lagrangian, one must keep in mind that $\mathcal{L}_\kappa(x,y)$ depends both on $P_\tau(x,y)$ and on its adjoint $P_\tau(x,y)^*$ (cf. (68)). Therefore, when applying the chain rule, we obtain contributions which are complex linear and complex anti-linear in $\delta P_\tau(x,y)$. We write the first variation with traces as

$$\delta\mathcal{L}_\kappa(x,y) = \mathrm{Tr}_{S_y}\big(B\,\delta P(x,y)\big) + \mathrm{Tr}_{S_x}\big(C\,\delta P(x,y)^*\big)$$

with linear operators $B : S_x \to S_y$ and $C : S_y \to S_x$. Since $\delta P(x,y)$ can be chosen arbitrarily, this equation uniquely defines both B and C. Since the variation of the Lagrangian is always real-valued, it follows that $C = B^*$. Using furthermore the symmetry of the Lagrangian in the arguments x and y, we conclude that the first variation of the Lagrangian can be written as (see also [8, Section 5.2])

$$\delta\mathcal{L}_\kappa(x,y) = \mathrm{Tr}_{S_y}\big(Q(y,x)\,\delta P(x,y)\big) + \mathrm{Tr}_{S_x}\big(Q(x,y)\,\delta P(x,y)^*\big) \tag{69}$$

with a kernel $Q(x,y) : S_y \to S_x$ which is symmetric in the sense that

$$Q(x,y)^* = Q(y,x)\,. \tag{70}$$

The EL equations are expressed in terms of the kernel $Q(x,y)$ as follows.

Proposition 4.2 (Euler-Lagrange equations) *Let ρ be a minimizer of the causal action principle. Then for a suitable choice of the Lagrange parameters λ and κ, the integral operator Q with kernel defined by (69) satisfies the equations*

$$\int_M Q(x,y)\,\psi^u(y)\,d\rho(y) = \frac{\lambda}{2}\,\psi^u(x) \qquad \text{for all } u \in \mathcal{H} \text{ and } x \in M\,. \tag{71}$$

We note for clarity that by writing the Eq. (71) we imply that the integral must exist and be finite.

Proof of Proposition 4.2 Using (69), the first variation of $\mathcal{S}_{\kappa,\lambda}$ is computed by

$$\begin{aligned}
&\delta\mathcal{S}_{\kappa,\lambda} \\
&= \iint_{M\times M} \Big(\mathrm{Tr}_{S_y}\big(Q(y,x)\,\delta P(x,y)\big) + \mathrm{Tr}_{S_x}\big(Q(x,y)\,\delta P(x,y)^*\big)\Big)\,d\rho(x)\,d\rho(y) \\
&\quad - \lambda \int_M \mathrm{Tr}\big(\delta P(x,x)\big)\,d\rho(x)\,.
\end{aligned}$$

Noting that $\delta P(x,y) = \delta P(y,x)$, after renaming the integration variables in the first summand of the double integral, we obtain

$$\begin{aligned} \delta \mathcal{S}_{\kappa,\lambda} = 2 \iint_{M \times M} & \mathrm{Tr}_{S_x} \big(Q(x,y)\, \delta P(y,x) \big) \\ & - \lambda \int_M \mathrm{Tr}_{S_x} \big(\delta P(x,x) \big)\, d\rho(x)\,. \end{aligned} \tag{72}$$

Next, we express δP in terms of the variation of the physical wave functions. By Lemma 1.3, we know that

$$P_\tau(x,y) = -\Psi_\tau(x) \Psi_\tau(y)^*\,.$$

Differentiating this relation gives

$$\delta P(x,y) = -(\delta \Psi)(x)\; \Psi(y)^* - \Psi(x)\; (\delta \Psi)(y)^*\,.$$

We now specialize to the case that the variation is trivial on the orthogonal complement of a one-dimensional subspace $I = \mathrm{span}(u) \subset \mathcal{H}$. Then for any $\phi \in S_y$,

$$\delta P(x,y)\, \phi = -\delta \psi^u(x)\, \prec \psi^u(y) \,|\, \phi \succ_y - \psi^u(x)\, \prec \delta \psi^u(y) \,|\, \phi \succ_y\,.$$

By inserting a phase factor according to

$$\delta \psi^u \to e^{i\varphi}\, \delta \psi^u\,,$$

one sees that $\delta \psi^u$ can be varied independently inside and outside the spin scalar product. Therefore, it suffices to consider variations inside the spin scalar product. Thus the vanishing of the first variation (72) yields the condition

$$0 = 2 \iint_{M \times M} \prec \delta \psi^u(x) \,|\, Q(x,y)\, \psi^u(y) \succ_x - \lambda \int_M \prec \delta \psi^u(x) \,|\, \psi^u(x) \succ_x\,.$$

Since the variation $\delta \psi^u$ is arbitrary (within the class of smooth and compactly supported variations), the result follows. □

We remark that the kernel $Q(x,y)$ also gives rise to an operator on the one-particle Krein space $(\mathcal{K}, <.|.>)$ as introduced in Sect. 1.5. Thus, in analogy to (24), one sets

$$Q\,:\, \mathcal{D}(Q) \subset \mathcal{K} \to \mathcal{K}\,, \qquad (Q\psi)(x) = \int_M Q(x,y)\, \psi(y)\, d\rho(y)\,,$$

where the domain $\mathcal{D}(Q)$ can be chosen for example as the continuous wave functions with compact support. The symmetry property of the kernel (70) implies

that the operator Q is symmetric on the Krein space $(\mathcal{K}, <.|.>)$. Equation (71) can be written in a compact form as the operator equation

$$\big(2Q - \lambda\, \mathbb{1}\big)\, \Psi = 0 \tag{73}$$

(where Ψ is again the wave evaluation operator (18)). In words, this equation means that the operator $(2Q - \lambda\, \mathbb{1})$ vanishes on the physical wave functions. However, the operator equation (73) is not satisfying mathematically because the physical wave functions in the image of Ψ are in general not vectors of the Krein space $(\mathcal{K}, <.|.>)$ (see Sect. 1.5). Nevertheless, (73) is useful as a short notation for the EL equations (71).

Remark 4.3 (more general variations) Clearly, only a special class of variations of the universal measure can be described by variations of the physical wave functions. As a consequence, the resulting EL equations (71) are only *necessary* conditions for ρ to be a critical point of the action (67). We now explain how these necessary conditions are related to the stronger EL equations as derived in [1].

As an example of variations which are not covered by the ansatz (64), one can multiply the universal measure by weight functions

$$d\rho_\tau = f_\tau\, d\rho\,, \tag{74}$$

where $(f_\tau)_{\tau \in (-\delta, \delta)}$ is a family of non-negative functions which are integrable and have mean zero, i.e.

$$f_\tau \geq 0 \qquad \text{and} \qquad \int_M f_\tau\, d\rho = 0\,.$$

Computing first variations of the action (67) gives rise to the equation

$$2 \int_M \mathcal{L}_\kappa(x, y)\, d\rho(y) + \lambda\, \mathrm{tr}(x) = \text{const} \qquad \text{on } M\,. \tag{75}$$

This is an additional EL equation which minimizers of the causal action principle must satisfy. It turns out that in the limiting case of an interacting system in Minkowski space (to be discussed in Sects. 5.2 and 5.3 below), this equation can be satisfied simply by a rescaling of the local correlation operators.

Variations of the physical wave functions as well as variations of the form (74) have the property that the support of the universal measure changes continuously (in the sense that for every compact set $K \subset \mathcal{F}$ and every open neighborhood U of $K \cap \text{supp}\, \rho$ there is $\varepsilon > 0$ such that $\text{supp}\, \rho_\tau \cap K \subset U$ for all τ with $|\tau| < \varepsilon$). Such variations can be regarded as the analogs of variations of the potentials, the metric or the wave functions in classical field theory or quantum mechanics. However, in the setting of causal fermion systems there are also more general smooth variations for which the support of the measure ρ_τ changes discontinuously. A typical example

is to let ρ be a bounded measure and to set

$$\rho_\tau = (1-\tau^2)\,\rho + \tau^2\,\rho(\mathcal{F})\,\delta_x\,, \tag{76}$$

where δ_x is the Dirac measure supported at $x \notin \operatorname{supp}\rho$. The EL equations corresponding to such variations have a different mathematical structure, which we cannot explain in detail here. Generally speaking, for interacting systems in Minkowski space, the EL equations of Proposition 4.2 give rise to an effective interaction via *classical* gauge fields (this so-called *continuum limit* will be discussed in Sect. 5.2). The EL equations corresponding to more general variations like (76), however, give rise to an effective interaction via bosonic *quantum* fields. We will come back to this point in Sect. 5.3. ◇

4.2 Symmetries and Conserved Surface Layer Integrals

In [20] it is shown that symmetries of the Lagrangian give rise to conservation laws. These results can be understood as adaptations of Noether's theorem to the causal action principle. Since the mathematical structure of the causal action principle is quite different from that of the Lagrangian formulation of classical field theory, these adaptations are not straightforward. We now explain a few concepts and results from [20] which are important for understanding the general physical picture.

We first recall that the conservation laws obtained from the classical Noether theorem state that the integral of a certain density over a Cauchy surface $\mathcal{N}$ does not depend on the choice of $\mathcal{N}$. For example, charge conservation states that the spatial integral of the charge density gives a constant. As another example, energy conservation states that in a static space-time background, the integral of the energy density is a constant. In general terms, the conserved quantities are spatial integrals over a Cauchy surface $\mathcal{N}$ (see the left of Fig. 1). In the setting of causal fermion systems, it is unclear how such surface integrals should be defined, in particular because we do not have a measure on hypersurfaces and because it is not clear what the normal ν on the hypersurface should be. This is the reason why in the Noether-like theorems in [20] one works instead of surface integrals with so-called

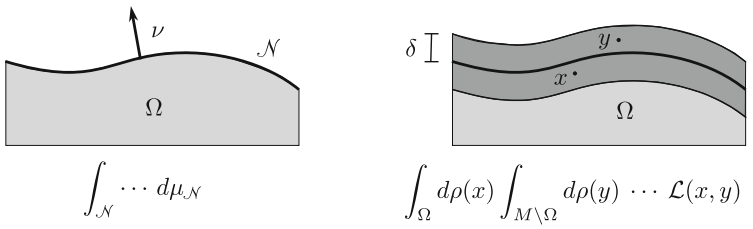


Fig. 1 A surface integral and a corresponding surface layer integral

surface layer integrals where one integrates over a boundary layer of a set $\Omega \subset M$ (see the right of Fig. 1). The width δ of this layer is the length scale on which $\mathcal{L}(x,y)$ decays. For a system composed of Dirac particles (similar as explained in Sect. 2 for the Minkowski vacuum and in Sect. 5.2 for interacting systems), this length scale can be identified with the *Compton scale* $\sim m^{-1}$ of the Dirac particles. Thus the width of the surface layer is a non-zero macroscopic length scale. In particular, the surface layer integrals cannot be identified with or considered as a generalization of the surface integrals of the classical Noether theorem. However, in most situations of interest, when the surface N is almost flat on the Compton scale (like for a spatial hyperplane in Minkowski space), the surface layer integral can be well-approximated by a corresponding surface integral. It turns out that in this limiting case, the conservation laws obtained from the Noether-like theorems in [20] go over to corresponding classical conservation laws.

From the conceptual point of view, the most interesting conservation law is *charge conservation*. In order to construct the underlying symmetry, we let $\mathcal{A}$ be a bounded symmetric operator on $\mathcal{H}$ and let

$$\mathcal{U}_\tau := \exp(i\tau \mathcal{A})$$

be the corresponding one-parameter family of unitary transformations. We introduce the family of transformations

$$\Phi_\tau : \mathcal{F} \to \mathcal{F}, \qquad \Phi_\tau(x) = \mathcal{U}_\tau\, x\, \mathcal{U}_\tau^{-1}.$$

Since the Lagrangian is defined via the spectrum of operators on $\mathcal{H}$, it clearly remains unchanged if all operators are unitarily transformed, i.e.

$$\mathcal{L}\big(\Phi_\tau(x), \Phi_\tau(y)\big) = \mathcal{L}(x,y). \tag{77}$$

In other words, the transformations Φ_τ describe a *symmetry of the Lagrangian*. Next, one constructs a corresponding one-family of universal measures by taking the push-forward,

$$\rho_\tau := (\Phi_\tau)_* \rho .$$

As a consequence of the symmetry (77), this variation of the universal measure leaves the action invariant. Under suitable differentiability assumptions, this symmetry gives rise to the identity

$$\frac{d}{d\tau} \int_\Omega d\rho(x) \int_{M\setminus\Omega} d\rho(y) \Big(\mathcal{L}\big(\Phi_\tau(x), y\big) - \mathcal{L}\big(\Phi_{-\tau}(x), y\big) \Big) \Big|_{\tau=0} = 0, \tag{78}$$

valid for any compact subset $\Omega \subset M$.

We now explain how the identity (78) is related to a conservation law. To this end, for simplicity we consider a system in Minkowski space (similar as explained

for the vacuum in Sect. 2) and choose a sequence of compact sets Ω_n which exhaust the region between two Cauchy surfaces at times $t = t_0$ and $t = t_1$. Then the surface layer integral (78) reduces to the difference of integrals over surface layers at times $t \approx t_0$ and $t \approx t_1$. Next, we choose $\mathcal{A} = \pi_{\langle u \rangle}$ as the projection operator on the one-dimensional subspace generated by a vector $u \in \mathcal{H}$. Then in the limit $\varepsilon \searrow 0$ in which the UV regularization is removed, the resulting surface layer integral at time $t \approx t_0$ reduces to the integral

$$\int_{\mathbb{R}^3} \prec u(t_0, \vec{x}) \,|\, \gamma^0 u(t_0, \vec{x}) \succ_{(t_0, \vec{x})} d^3x \,,$$

thereby reproducing the probability integral in Dirac theory. As a consequence, the representation of the scalar product $\langle .|. \rangle_{\mathcal{H}}$ as an integral over a Cauchy surface (26) has a natural generalization to the setting of causal fermion systems, if the surface integral is replaced by a corresponding surface layer integral. This result also shows that the spatial normalization of the fermionic projector (where one works with spatial integrals of the form (47); for details see [28]) really is the correct normalization method which reflects the intrinsic conservation laws of the causal fermion system.

The conservation laws in [20] also give rise to the *conservation of energy and momentum*, as we now outline. In the classical Noether theorem, these conservation laws are a consequence of space-time symmetries as described most conveniently using the notion of Killing fields. Therefore, one must extend this notion to the setting of causal fermion systems. Before explaining how this can be accomplished, we recall the procedure in the classical Noether theorem: In the notion of a Killing field, one distinguishes the background geometry from the additional particles and fields. The background geometry must have a symmetry as described by the Killing equation. The additional particles and fields, however, do not need to have any symmetries. Nevertheless, one can construct a symmetry of the whole system by actively transporting the particles and fields along the flow lines of the Killing field. The conservation law corresponding to this symmetry transformation gives rise to the conservation of energy and momentum.

In a causal fermion system, there is no clear-cut distinction between the background geometry and the particles and fields of the system, because all of these structures are encoded in the underlying causal fermion system and mutually depend on each other. Therefore, instead of working with a symmetry of the background geometry, we work with the notion of an approximate symmetry. By actively transforming those physical wave functions which do not respect the symmetry, such an approximate symmetry again gives rise to an exact symmetry transformation, to which the Noether-like theorems in [20] can be applied. More precisely, one begins with a C^1-family of transformations $(f_\tau)_{\tau \in (-\delta, \delta)}$ of space-time,

$$f_\tau \,:\, M \to M \qquad \text{with} \qquad f_0 = \mathbb{1} \,, \tag{79}$$

which preserve the universal measure in the sense that $(f_\tau)_* \rho = \rho$. The family (f_τ) can be regarded as the analog of a flow in space-time along a classical Killing field.

Moreover, one considers a family of unitary transformations $(\mathcal{U}_\tau)_{\tau \in (-\delta,\delta)}$ on $\mathcal{H}$ with the property that

$$\mathcal{U}_{-\tau}\, \mathcal{U}_\tau = \mathbb{1} \qquad \text{for all } \tau \in (-\delta, \delta)\,.$$

Combining these transformations should give rise to an *approximate symmetry* of the wave evaluation operator (18) in the sense that if we compare the transformation of the space-time point with the unitary transformation by setting

$$E_\tau(u,x) := (\Psi u)\big(f_\tau(x)\big) - (\Psi \mathcal{U}_\tau^{-1} u)(x) \qquad (x \in M, u \in \mathcal{H})\,, \tag{80}$$

then the operator $E_\tau : \mathcal{H} \to C^0(M, SM)$ should be sufficiently small. Here "small" means for example that E vanishes on the orthogonal complement of a finite-dimensional subspace of $\mathcal{H}$; for details see [20, Section 6]. Introducing the variation Φ_τ by

$$\Phi_\tau : M \to \mathcal{F}\,, \qquad \Phi_\tau(x) = \mathcal{U}_\tau\, x\, \mathcal{U}_\tau^{-1}\,,$$

we again obtain a symmetry of the Lagrangian (77). This gives rise to conserved surface layer integrals of the form (78). In order to bring these surface layer integrals into a computable form, one decomposes the first variation of Φ_τ as

$$\delta\Phi(x) := \partial_\tau \Phi_\tau(x)\big|_{\tau=0} = \delta f(x) + v(x)\,, \tag{81}$$

where δf is the first variation of f_τ, (79), and $v(x)$ is a vector field on $\mathcal{F}$ along M which is transversal to $M \subset \mathcal{F}$. Expressing v in terms of the operator E in (80) shows that v is again small, making it possible to compute the corresponding variation of the Lagrangian in (78). We remark that in the decomposition (81), the vector field δf describes a transformation of the space-time points. The vector field v, however, can be understood as an active transformation of all the objects in space-time which do *not* have the space-time symmetry (similar as described above for the parallel transport of the particles and fields along the flow lines of the Killing field in the classical Noether theorem).

In order to get the connection to classical conservation laws, one again studies a system in Minkowski space and considers the limiting case where a sequence Ω_n exhausts the region between two Cauchy surfaces at times $t = t_0$ and $t = t_1$. In this limiting case, the conserved surface layer integral reduces to the surface integral

$$\int_{\mathbb{R}^3} T_{i0}\, K^i\, d^3x\,,$$

where T_{ij} is the energy-momentum tensor of the Dirac particles and $K = \delta f$ is a Killing field. This shows that the conservation of energy and momentum is a special case of more general conservation laws which are intrinsic to causal fermion systems.

4.3 The Initial Value Problem and Time Evolution

In order to get a better understanding of the dynamics described by the causal action principle, it is an important task to analyze the initial value problem. The obvious questions are: What is the initial data? Is it clear that a solution exists? Is the solution unique? How do solutions look like? Giving general answers to these questions is a difficult mathematical problem. In order to evaluate the difficulties, one should recall that ρ describes space-time as well as all structures therein. Therefore, similar as in the Cauchy problem for the Einstein equations, solving the initial value problem involves finding the geometry of space-time together with the dynamics of all particles and fields. In view of the complexity of this problem, the only results known at present are contained in the paper [15], where an initial value problem is formulated and some existence and uniqueness theorems are proven. We now review a few methods and results of this paper. Moreover, at the end of this section we mention an approach proposed in [19] for obtaining more explicit information on the dynamics by analyzing perturbations of a given minimizing measure.

Since the analysis of the causal action principle is technically demanding, in [15] one considers instead so-called *causal variational principles in the compact setting*. In order to get into this simplified setting, one replaces $\mathcal{F}$ by a compact metric space (or a smooth manifold). The Lagrangian is replaced by a non-negative continuous function $\mathcal{L} \in C^{0,1}(\mathcal{F} \times \mathcal{F}, \mathbb{R}_0^+)$ which is symmetric in its two arguments. Similar to (2) one minimizes the action

$$\mathcal{S}(\rho) = \iint_{\mathcal{F}\times\mathcal{F}} \mathcal{L}(x,y)\, d\rho(x)\, d\rho(y)$$

in the class of all normalized regular Borel measures on $\mathcal{F}$, but now leaving out the constraints (4) and (5). Space-time is again defined by $M := \operatorname{supp} \rho$. The resulting causal structure is defined by saying that two space-time points $x, y \in M$ are called *timelike* separated if $\mathcal{L}(x,y) > 0$, and *spacelike* separated if $\mathcal{L}(x,y) = 0$. Clearly, in this setting there are no wave functions. Nevertheless, causal variational principles in the compact setting incorporate basic features of the causal action principle and are therefore a good starting point for the analysis (for a more detailed introduction and structural results on the minimizing measures see [26]).

When solving the classical Cauchy problem, instead of searching for a global solution, it is often easier to look for a local solution around a given initial value surface. This concept of a local solution also reflects the common physical situation where the physical system under consideration is only a small subsystem of the whole universe. With this in mind, we would like to "localize" the variational principle to a subset $\mathfrak{I} \subset \mathcal{F}$, referred to as the *inner region*. There is the complication that the Lagrangian $\mathcal{L}(x,y)$ is nonlocal in the sense that it may be non-zero for points $x \in \mathfrak{I}$ and $y \in \mathcal{F} \setminus \mathfrak{I}$. In order to take this effect into account, one describes the influence of the "outer region" $\mathcal{F} \setminus \mathfrak{I}$ by a so-called *external potential* $\phi : \mathcal{F} \to \mathbb{R}_0^+$. In the limiting case when the outer region becomes large, this gives rise to the so-

called *inner variational principle*, where the action defined by

$$\mathcal{S}_{\mathfrak{J}}[\rho, \phi] = \iint_{\mathfrak{J}\times\mathfrak{J}} \mathcal{L}(x,y)\, d\rho(x)\, d\rho(y) + 2 \int_{\mathfrak{J}} \big(\phi(x) - \mathfrak{s}\big)\, d\rho(x) \tag{82}$$

is minimized under variations of ρ in the class of regular Borel measures on $\mathfrak{J}$ (not necessarily normalized because the volume constraint is now taken care of by the corresponding Lagrange parameter $\mathfrak{s} > 0$).

The *initial values* are described by a regular Borel measure ρ_0 (which is to be thought of as the universal measure restricted to a time slice around the initial value surface in space-time). The *initial conditions* are implemented by demanding that

$$\rho \geq \rho_0 \,. \tag{83}$$

The naive method of minimizing (82) under the constraint (83) is not a sensible concept because the constraint (83) would give rise to undesirable Lagrange multiplier terms in the EL equations. Instead, one minimizes (82) without constraints, but chooses the external potential ϕ in such a way that the minimizing measure satisfies the initial values (83). It turns out that this procedure does not determine the external potential uniquely. Therefore, the method proposed in [15] is to *optimize the external potential* by making it in a suitable sense "small." As is made precise in [15] in various situations, the resulting interplay between minimizing the action and optimizing the external potential gives rise to unique solutions of the initial-value problem with an optimal external potential.

We point out that, due to the mathematical simplifications made, the results in [15] do not apply to physically interesting situations like the initial value problem for interacting Dirac sea configurations. Moreover, the methods in [15] do not seem to give explicit information on the dynamics of causal fermion systems. Therefore, it is a promising complementary approach to consider perturbations of a given minimizing measure (which should describe the "vacuum configuration") and to analyze the dynamics of the perturbations by studying the resulting EL equations. This approach is pursued in [19] in the following way. In order to describe the perturbations of the minimizing measure ρ, one considers smooth variations for which the support of ρ changes continuously. Combining (64) and (74), these variations can be written as

$$\tilde{\rho}_\tau = (F_\tau)_* \big(f_\tau\, \rho\big)$$

with a family of mappings $F_\tau : M \to \mathcal{F}$ and a family of non-negative functions f_τ. Expanding in powers of τ, these variations can be described conveniently in terms of sections of *jet bundles* over M. The EL equations yield conditions on the jets, which can be rewritten as dynamical equations in space-time.

5 Limiting Cases

We now discuss different limiting cases of causal fermion systems.

5.1 The Quasi-free Dirac Field and Hadamard States

We now turn attention to interacting systems. The simplest interaction is obtained by inserting an *external potential* into the Dirac equation (25),

$$\big(i\gamma^j \partial_j + \mathcal{B} - m\big)\, \psi(x) = 0\,. \tag{84}$$

Another situation of physical interest is to consider the Dirac equation in an external classical gravitational field as described mathematically by a globally hyperbolic Lorentzian manifold $(\mathscr{M}, g)$. In this section, we explain how the methods and results of Sect. 2 generalize to the situation when an external field is present. This will also give a connection to quasi-free Dirac fields and Hadamard states. In order to keep the explanations as simple as possible, we here restrict attention to an external potential $\mathcal{B}$ in Minkowski space, but remark that many methods and results could or have been worked out also in the presence of a gravitational field.

The obvious conceptual difficulty when extending the constructions of Sect. 2 is that one no longer has the notion of "negative-frequency solutions" which were essential for introducing Dirac sea configurations (see Lemma 2.8). In order to overcome this difficulty, one needs to decompose the solution space of the Dirac equation (84) into two subspace, in such a way that without external potential the two subspaces reduce to the subspaces of positive and negative frequency. This *external field problem* was solved perturbatively in [7, 16] and non-perturbatively in [23–25] (for a more detailed exposition see [8, §2.1]).

We now briefly outline the non-perturbative treatment, which relies on the construction on the so-called *fermionic signature operator*. Choosing again the scalar product (26), the solution space of the Dirac equation (84) forms a Hilbert space denoted by $(\mathcal{H}_m, (.|.)_m)$. Moreover, on the Dirac wave functions (not necessarily solutions of the Dirac equations) one may introduce a dual pairing by integrating the spin scalar product over all of space-time,

$$<.|.> \;:\; C^\infty(\mathscr{M}, S\mathscr{M}) \times C_0^\infty(\mathscr{M}, S\mathscr{M}) \to \mathbb{C}\,, \quad <\psi|\phi> = \int_{\mathscr{M}} \prec\psi|\phi\succ_x d^4x\,. \tag{85}$$

The basic idea is to extend this dual pairing to a bilinear form on the Hilbert space $\mathcal{H}_m$ and to represent this bilinear form in terms of the Hilbert space scalar product

$$<\phi_m|\psi_m> = (\phi_m \,|\, \mathcal{S}\, \psi_m)_m\,.$$

If $\mathscr{M}$ is a space-time of *finite lifetime*, this construction can indeed be carried out and defines the *fermionic signature operator* $\mathcal{S}$ being a bounded symmetric operator on $\mathcal{H}_m$ (see [25]). The positive and negative spectral subspaces of $\mathcal{S}$ give the desired decomposition of $\mathcal{H}_m$ into two subspaces. We remark that the fermionic signature operator makes it possible to study *spectral geometry* for Lorentzian signature (see [22] and [12] for the connection to index theory).

In space-times of infinite lifetime like Minkowski space, the above method does not work because (85) does not extend to a continuous bilinear form on $\mathcal{H}_m \times \mathcal{H}_m$. The underlying problem is that the time integral in (85) in general diverges for solutions of the Dirac equation. In order to circumvent this problem, one considers families of Dirac solutions $(\psi_m)_{m \in I}$ (for an open interval $I = (m_a, m_b) \subset (0, \infty)$) and makes use of the fact that integrating over the mass parameter generates decay of the wave functions for large times (for details see [24]). As a result, one can make sense of the equation

$$< \int_I \psi_m \, dm \,|\, \int_I \psi_{m'} \, dm' > \;=\; \int_I (\psi_m \,|\, \mathcal{S}_m \, \phi_m)_m \, dm \,,$$

which uniquely defines a family of bounded symmetric operators $(\mathcal{S}_m)_{m \in I}$. Now the positive and negative spectral subspaces of the operator $\mathcal{S}_m$ again give the desired decomposition of $\mathcal{H}_m$ into two subspaces.

Having decomposed the solution space, one may choose the Hilbert space $\mathcal{H}$ of the causal fermion system as one of the two subspaces of the solution space. Choosing an orthonormal basis (u_ℓ) of $\mathcal{H}$ and introducing the unregularized kernel of the fermionic projector again by (43), one obtains a two-point distribution $P(x, y)$. Using that this two-point distribution comes from a projection operator in the Hilbert space $\mathcal{H}_m$, there is a canonical construction which gives a quasi-free Dirac field together with a Fock representation such that the two-point distribution coincides with $P(x, y)$. In the language of algebraic quantum field theory, this result is stated as follows (see [23, Theorem 1.4]):

Theorem 5.1 *There is an algebra of smeared fields generated by* $\Psi(g)$, $\Psi^*(f)$ *together with a quasi-free state* ω *with the following properties:*

(a) The canonical anti-commutation relations hold:

$$\{\Psi(g), \Psi^*(f)\} = <g^* \,|\, \tilde{k}_m f> \,, \qquad \{\Psi(g), \Psi(g')\} = 0 = \{\Psi^*(f), \Psi^*(f')\} \,.$$

(b) The two-point function of the state is given by

$$\omega\big(\Psi(g)\, \Psi^*(f)\big) = - \iint_{\mathscr{M} \times \mathscr{M}} g(x) P(x, y) f(y) \, d^4x \, d^4y \,.$$

This theorem means that before introducing an UV regularization, the description of the Dirac system using the fermionic projector is equivalent to the usual description of a quasi-free Dirac field in quantum field theory.

Moreover, it is shown in [23] that the two-point distribution $P(x, y)$ is of *Hadamard form*, provided that $\mathcal{B}$ is smooth, not too large and decays faster than quadratically for large times (for details see [23, Theorem 1.3] and the references in this paper). This result implies that the representation of the quasi-free Dirac field as obtained from the fermionic projector is a suitable starting point for a perturbative treatment of the resulting interacting theory (see for example [4]).

In our context, the fact that $P(x, y)$ is of Hadamard form implies that the results in Sect. 1.2 also apply in the presence of an external potential, as we now explain. The Hadamard property means in words that the bi-distribution $P(x, y)$ in the presence of the external potential has the same singularity structure as in the Minkowski vacuum. As a consequence, the arguments in Sect. 1.2 remain true if the points x and y are sufficiently close to each other. More precisely, the relevant length scale is given by the inverse of the amplitude $|\mathcal{B}(x)|^{-1}$ of the external potential. On the other hand, the separation of the points x and y must be larger than the scale ε on which regularization effects come into play. Therefore, the causal structure of a causal fermion system agrees with that of Minkowski space on the scale $\varepsilon \ll \left|x^0 - y^0\right| + \left|\vec{x} - \vec{y}\right| \ll |\mathcal{B}|^{-1}$ (where $|\mathcal{B}|$ is any matrix norm). Thinking of ε as being at least as small as the Planck length, in most situations of interest the lower bound is no restriction. The upper bound is also unproblematic because the causal structure on the macroscopic scale can still be recovered by considering paths in space-time and subdividing the path on a scale $\delta \ll |\mathcal{B}|^{-1}$ (similar as explained in [14, Section 4.4] for the spin connection). With this in mind, we conclude that the causal structure of a causal fermion system indeed agrees with that of Minkowski space, even in the presence of an external potential.

5.2 *Effective Interaction via Classical Gauge Fields*

We now outline how to describe interacting systems in Minkowski space by analyzing the EL equations corresponding to the causal action principle as worked out in Proposition 4.2. In this so-called *continuum limit* the interaction is described by classical gauge fields. For brevity, we can only explain a few basic concepts and refer the interested reader to the detailed computations in the book [6].

Let us begin with the Minkowski vacuum. As shown in Sect. 2.2, regularizing a vacuum Dirac sea configuration gives rise to a causal fermion system $(\mathcal{H}, \mathcal{F}, \rho^\varepsilon)$. Moreover, we saw in the following Sects. 2.3 and 2.4 that the inherent structures of the causal fermion system can be identified with those of Minkowski space (in particular, see (37) as well as Propositions 2.6 and 2.7). This makes it possible to write the EL equations (71) as

$$\int_{\mathscr{M}} Q^\varepsilon(x, y) \left(\mathfrak{R}_\varepsilon u_\ell\right)(y)\, d^4y = \frac{\lambda}{2} \left(\mathfrak{R}_\varepsilon u_\ell\right)(x) \qquad \text{for all } u \in \mathcal{H}\,, \tag{86}$$

where the regularized kernel $Q^\varepsilon(x,y)$ is again defined via (69) as the derivative of the Lagrangian. Next, one chooses the Hilbert space $\mathcal{H}$ as in Sect. 2.5 as the Dirac sea configuration formed of all negative-energy solutions of the Dirac equation. Then $P^\varepsilon(x,y)$ can be computed explicitly by regularizing the distribution $P(x,y)$ as given in momentum space by (46) and in position space by (48) and Lemma 2.9. Computing $Q^\varepsilon(x,y)$, it turns out that the EL equations are mathematically well-defined if the convolution integral in (86) is rewritten with the help of Plancherel's theorem as a multiplication in momentum space. The analysis of the *continuum limit* gives a procedure for studying these equations in the asymptotics $\varepsilon \searrow 0$ when the regularization is removed. The effective equations obtained in this asymptotic limit are evaluated most conveniently in a formalism in which the unknown microscopic structure of space-time (as described by the regularization) enters only in terms of a finite (typically small) number of so-called *regularization parameters*. According to the method of variable regularization (see Remark 2.1), one needs to analyze the dependence of the regularization parameters in detail. It turns out that the causal fermion systems obtained from the vacuum Dirac sea configuration satisfy the EL equations in the continuum limit, for any choice of the regularization parameters.

The first step towards interacting systems is to consider systems involving *particles* and/or *anti-particles*. To this end, one simply modifies the constructions in Sect. 2.5 by choosing the Hilbert space $\mathcal{H}$ differently. Namely, instead of choosing all negative-energy solutions, one chooses $\mathcal{H}$ as a subspace of the solution space which differs from the space of all negative-energy solutions by a finite-dimensional subspace. In other words, $\mathcal{H}$ is obtained from the space of all negative-energy solutions by taking out a finite number n_a of states and by adding a finite number of states n_p of positive energy. Thus, denoting the regularized kernel of the fermionic projector of the Minkowski vacuum for clarity by $P^\varepsilon_\text{sea}(x,y)$, the kernel of the fermionic projector (42) can be written as

$$\begin{aligned} P^\varepsilon(x,y) &= P^\varepsilon_\text{sea}(x,y) \\ &\quad - \sum_{k=1}^{n_\text{p}} \big(\mathfrak{R}_\varepsilon \psi_k\big)(x) \overline{\big(\mathfrak{R}_\varepsilon \psi_k\big)(y)} + \sum_{l=1}^{n_\text{a}} \big(\mathfrak{R}_\varepsilon \phi_l\big)(x) \overline{\big(\mathfrak{R}_\varepsilon \phi_l\big)(y)}\,, \end{aligned} \tag{87}$$

where ψ_k and ϕ_l are suitably normalized bases of the particle and anti-particle states, respectively. In this procedure, we again take Dirac's concept of a "sea" of particles literally and describe particles and anti-particles by occupying positive-energy states and creating "holes" in the Dirac sea, respectively. We also remark that the construction (87) modifies the kernel of the fermionic projector only by smooth contributions and thus preserves the singularity structure of $P^\varepsilon(x,y)$ as $\varepsilon \searrow 0$. As a consequence, the correspondence of the inherent structures of the causal fermion systems to the structures in Minkowski space remains unchanged (just as explained at the end of Sect. 5.1 for an external potential).

According to (87), the particle and anti-particle states modify the kernel of the fermionic projector. It turns out that this has the effect that the EL equations in the

continuum limit no longer hold. In order to again satisfy these equations, we need to introduce an interaction. In mathematical terms, this means that the universal measure ρ must be modified. The basic question is how to modify the universal measure in such a way that the EL equations in the continuum limit again hold. It turns out that it is a useful first step to insert an external potential $\mathcal{B}$ into the Dirac equation (25) by going over to the Dirac equation (84). Choosing $\mathcal{H}$ as a subspace of the solution space of this Dirac equation, the constructions of Sect. 2 again apply and give rise to causal fermion systems $(\mathcal{H}, \mathcal{F}, \rho^\varepsilon)$. The potential $\mathcal{B}$ modifies the dynamics of all physical wave functions in a collective way. Now one can ask the question whether the resulting causal fermion systems satisfy the EL equations in the continuum limit. It turns out that this is the case if and only if the potential $\mathcal{B}$ satisfies certain equations, which can be identified with classical field equations for the potential $\mathcal{B}$. In this way, the causal action principle gives rise to classical field equations. In order to make our concepts clear, we point out that the potential $\mathcal{B}$ merely is a convenient device in order to describe the collective behavior of all physical wave functions. It should not be considered as a fundamental object of the theory. We also note that, in order to describe variations of the physical wave functions, the potential in (84) can be chosen arbitrarily (in particular, the potential does not need to satisfy any field equations). Each choice of $\mathcal{B}$ describes a different variation of the physical wave functions. It is the EL equations in the continuum limit which single out the physically admissible potentials as being those which satisfy the field equations.

Before going on, we briefly explain how the subspace $\mathcal{H}$ is chosen. Clearly, the Dirac equation (84) cannot in general be solved in closed form. Therefore, for an explicit analysis one must use perturbative methods. When performing the perturbation expansion, one must be careful about the proper normalization of the fermionic states (in the sense that spatial integrals of the form (47) should be preserved). Moreover, one must make sure that the singular structure of $P(x, y)$ in position space is compatible with the causal action principle (meaning that the light-cone expansion of $P(x, y)$ only involves bounded integrals of $\mathcal{B}$ and its derivatives). Satisfying these two requirements leads to the *causal perturbation expansion* (see [28] and the references therein). We also mention that regularizing the perturbation expansion is a delicate issue. This can already be understood for the simple regularization by mollification in Example 2.4, in which case it is not clear whether one should first mollify and then introduce the interaction or vice versa. The correct method for regularizing the perturbation expansion is obtained by demanding that the behavior under gauge transformations should be preserved by the regularization. This leads to the *regularized causal perturbation expansion* as developed in [8, Appendix D] and [6, Appendix F].

We proceed with a brief overview of the results of the analysis of the continuum limit. In [6] the continuum limit is worked out in several steps beginning from simple systems and ending with a system realizing the fermion configuration of the standard model. For each of these systems, the continuum limit gives rise to effective equations for second-quantized fermion fields coupled to classical bosonic gauge fields (for the connection to second-quantized bosonic fields see Sect. 5.3 below).

To explain the structure of the obtained results, it is preferable to first describe the system modelling the leptons as analyzed in [6, Chapter 4]. The input to this model is the configuration of the leptons in the standard model without interaction. Thus the fermionic projector of the vacuum is assumed to be composed of three generations of Dirac particles of masses $m_1, m_2, m_3 > 0$ (describing e, μ, τ) as well as three generations of Dirac particles of masses $\tilde{m}_1, \tilde{m}_2, \tilde{m}_3 \geq 0$ (describing the corresponding neutrinos). Furthermore, we assume that the regularization of the neutrinos breaks the chiral symmetry (implying that we only see their left-handed components). We point out that the definition of the model does not involve any assumptions on the interaction.

The detailed analysis in [6, Chapter 4] reveals that the effective interaction in the continuum limit has the following structure. The fermions satisfy the Dirac equation coupled to a left-handed SU(2)-gauge potential $A_L = \big(A_L^{ij}\big)_{i,j=1,2}$,

$$\left[i\partial\!\!\!/ + \begin{pmatrix} A\!\!\!/_L^{11} & A\!\!\!/_L^{12}\, U_{\text{MNS}}^* \\ A\!\!\!/_L^{21}\, U_{\text{MNS}} & -A\!\!\!/_L^{11} \end{pmatrix} \chi_L - mY \right] \psi = 0\,,$$

where we used a block matrix notation (in which the matrix entries are 3×3-matrices). Here mY is a diagonal matrix composed of the fermion masses,

$$mY = \text{diag}(\tilde{m}_1, \tilde{m}_2, \tilde{m}_3,\ m_1, m_2, m_3)\,, \tag{88}$$

and U_{MNS} is a unitary 3×3-matrix (taking the role of the Maki-Nakagawa-Sakata matrix in the standard model). The gauge potentials A_L satisfy a classical Yang-Mills-type equation, coupled to the fermions. More precisely, writing the isospin dependence of the gauge potentials according to $A_L = \sum_{\alpha=1}^{3} A_L^\alpha \sigma^\alpha$ in terms of Pauli matrices, we obtain the field equations

$$\partial^k \partial_l (A_L^\alpha)^l - \Box (A_L^\alpha)^k - M_\alpha^2\, (A_L^\alpha)^k = c_\alpha\, \overline{\psi} \big(\chi_L \gamma^k\, \sigma^\alpha \big) \psi\,, \tag{89}$$

valid for $\alpha = 1, 2, 3$ (for notational simplicity, we wrote the Dirac current for one Dirac particle; for a second-quantized Dirac field, this current is to be replaced by the expectation value of the corresponding fermionic field operators). Here M_α are the bosonic masses and c_α the corresponding coupling constants. The masses and coupling constants of the two off-diagonal components are equal, i.e. $M_1 = M_2$ and $c_1 = c_2$, but they may be different from the mass and coupling constant of the diagonal component $\alpha = 3$. Generally speaking, the mass ratios M_1/m_1, M_3/m_1 as well as the coupling constants c_1, c_3 depend on the regularization. For a given regularization, they are computable.

Finally, our model involves a gravitational field described by the Einstein equations

$$R_{jk} - \frac{1}{2}\, R\, g_{jk} + \Lambda\, g_{jk} = \kappa\, T_{jk}\,, \tag{90}$$

where R_{jk} denotes the Ricci tensor, R is scalar curvature, and T_{jk} is the energy-momentum tensor of the Dirac field. Moreover, κ and Λ denote the gravitational and the cosmological constants, respectively. We find that the gravitational constant scales like $\kappa \sim \delta^{-2}$, where $\delta \geq \varepsilon$ is the length scale on which the chiral symmetry is broken.

In [6, Chapter 5] a system is analyzed which realizes the configuration of the leptons and quarks in the standard model. The result is that the field equation (89) is replaced by field equations for the electroweak and strong interactions after spontaneous symmetry breaking (the dynamics of the corresponding Higgs field has not yet been analyzed). Furthermore, the system again involves gravity (90).

A few clarifying remarks are in order. First, the above field equations come with corrections which for brevity we cannot discuss here (see [6, Sections 3.8, 4.4 and 4.6]). Next, it is worth noting that, although the states of the Dirac sea are explicitly taken into account in our analysis, they do not enter the field equations. More specifically, in a perturbative treatment, the divergences of the Feynman diagram describing the vacuum polarization drop out of the EL equations of the causal action. Similarly, the naive "infinite negative energy density" of the sea drops out of the Einstein equations, making it unnecessary to subtract any counter terms. We finally remark that the only free parameters of the theory are the masses in (88) as well as the parameter δ which determines the gravitational constant. The coupling constants, the bosonic masses and the mixing matrices are functions of the regularization parameters which are unknown due to our present lack of knowledge on the microscopic structure of space-time. The regularization parameters cannot be chosen arbitrarily because they must satisfy certain relations. But except for these constraints, the regularization parameters are currently treated as free empirical parameters.

To summarize, the dynamics in the continuum limit is described by Dirac spinors coupled to classical gauge fields and gravity. The effective continuum theory is manifestly covariant under general coordinate transformations. The only limitation of the continuum limit is that the bosonic fields are merely classical. We shall come back to second-quantized bosonic fields in Sect. 5.3 below.

5.3 Effective Interaction via Bosonic Quantum Fields

In Sect. 5.2 it was outlined that and in which sense the regularized Dirac sea vacuum satisfies the EL equations (71). In simple terms, these results mean that the regularized Dirac sea vacuum is a critical point of the causal action under variations of the physical wave functions (see Definition 4.1). We now explain why the regularized Dirac sea vacuum is *not a minimizer* of the causal action principle. This argument will lead us to a method for further decreasing the causal action. It also gives some insight on the structure of the minimizing measure. In particular, we shall see that the effective interaction in the resulting space-time is to be described effectively by bosonic *quantum* fields.

Suppose that $(\mathcal{H}, \mathcal{F}, \rho)$ is a causal fermion system describing a regularized Dirac sea configuration (see Sect. 2.5). In order to explain the basic idea, it suffices to consider the case that ρ has finite total volume (which can be arranged for example by considering the system in a four-dimensional box). For a unitary transformation $V \in \mathrm{U}(\mathcal{H})$, we define the measure $V(\rho)$ by

$$(V\rho)(\Omega) = \rho(V \Omega V^{-1}) \,. \tag{91}$$

We choose a finite number of unitary transformations $V_1, \ldots, V_L$ and introduce a new measure $\tilde{\rho}$ as the convex combination of the unitarily transformed measures,

$$\tilde{\rho} = \frac{1}{L} \sum_{\mathfrak{a}=1}^{L} V_{\mathfrak{a}} \rho \,.$$

Obviously, all linear constraints like the volume constraint (3) and the trace constraint (4) are preserved by this transformation. The action becomes

$$\begin{aligned} \mathcal{S}(\tilde{\rho}) &= \frac{1}{L^2} \sum_{\mathfrak{a},\mathfrak{b}=1}^{L} \iint_{\mathcal{F}\times\mathcal{F}} \mathcal{L}(x,y)\, d(V_{\mathfrak{a}}\rho)(x)\, d(V_{\mathfrak{b}}\rho)(y) \\ &= \frac{\mathcal{S}(\rho)}{L} + \frac{1}{L^2} \sum_{\mathfrak{a}\neq\mathfrak{b}} \iint_{\mathcal{F}\times\mathcal{F}} \mathcal{L}(x,y)\, d(V_{\mathfrak{a}}\rho)(x)\, d(V_{\mathfrak{b}}\rho)(y) \,. \end{aligned} \tag{92}$$

Due to the factor $1/L$, the first summand becomes small as L increases. The second summand involves all the contributions for $\mathfrak{a} \neq \mathfrak{b}$. If we can arrange that these contributions become small, then the action of the new measure $\tilde{\rho}$ will indeed be smaller than the action of ρ.

Let us consider the contributions for $\mathfrak{a} \neq \mathfrak{b}$ in more detail. In order to simplify the explanations, it is convenient to assume that the measures $V_{\mathfrak{a}}\rho$ have mutually disjoint supports (this can typically be arranged by a suitable choice of the unitary transformations $V_{\mathfrak{a}}$). Then the space-time $\tilde{M} := \operatorname{supp} \tilde{\rho}$ can be decomposed into L "sub-space-times" $M_{\mathfrak{a}} := \operatorname{supp} \rho_{\mathfrak{a}}$,

$$\tilde{M} = M_1 \cup \cdots \cup M_L \qquad \text{and} \qquad M_{\mathfrak{a}} \cap M_{\mathfrak{b}} = \varnothing \quad \text{if } \mathfrak{a} \neq \mathfrak{b} \,.$$

Likewise, a physical wave function ψ^u can be decomposed into the contributions in the individual sub-space-times,

$$\psi^u = \sum_{\mathfrak{a}=1}^{L} \psi^u_{\mathfrak{a}} \qquad \text{with} \qquad \psi^u_{\mathfrak{a}} := \chi_{M_{\mathfrak{a}}}\, \psi^u$$

(and $\chi_{M_{\mathfrak{a}}}$ is the characteristic function). This also gives rise to a corresponding decomposition of the fermionic projector:

Lemma 5.2 *Every sub-space-time $M_\mathfrak{a}$ of $\tilde{M}$ is homeomorphic to M, with a homeomorphism given by*

$$\phi_\mathfrak{a} \,:\, M \to M_\mathfrak{a}\,, \qquad \phi_\mathfrak{a}(x) := V_\mathfrak{a}^*\, x\, V_\mathfrak{a}\,.$$

Moreover, the mapping

$$V_\mathfrak{a}^*\big|_{S_x} \,:\, S_x \to S_{\phi_\mathfrak{a}(x)} \tag{93}$$

is an isomorphism of the corresponding spinor spaces. Identifying the spinor spaces in different sub-space-times via this isomorphism, the fermionic projector can be written as

$$P(x,y) = -\sum_{\mathfrak{a},\mathfrak{b}=1}^{L} \chi_{M_\mathfrak{a}}(x)\, P_{\mathfrak{a},\mathfrak{b}}(x,y)\, \chi_{M_\mathfrak{b}}(y) \qquad \text{with} \tag{94}$$

$$P_{\mathfrak{a},\mathfrak{b}}(x,y) := \Psi(x)\, V_\mathfrak{a}\, V_\mathfrak{b}^*\, \Psi(y)^*\,. \tag{95}$$

Proof The definition of $V\rho$, (91), immediately implies that the transformation (16) maps M to $M_\mathfrak{a}$ and is a homeomorphism. By definition of the physical wave function (16),

$$\psi^u(\phi_\mathfrak{a}(x)) = \pi_{\phi_\mathfrak{a}(x)} = \pi_{V_\mathfrak{a}^* x V_\mathfrak{a}} u = V_\mathfrak{a}^*\, \pi_x\, V_\mathfrak{a} u\,.$$

The identification (93) makes it possible to leave out the factor $V_\mathfrak{a}^*$. Then we can write the wave evaluation operator (18) as

$$\tilde{\Psi}(x) = \sum_{\mathfrak{a}=1}^{L} \chi_{M_\mathfrak{a}}(x)\, \Psi(x)\, V_\mathfrak{a}\,.$$

Applying (20) gives the result. □

This lemma makes it possible to rewrite the action (92) as

$$\mathcal{S}(\tilde{\rho}) = \frac{\mathcal{S}(\rho)}{L} + \frac{1}{L^2} \sum_{\mathfrak{a}\neq\mathfrak{b}} \iint_{M\times M} \mathcal{L}\big[P_{\mathfrak{a},\mathfrak{b}}(x,y)\big]\, d\rho(x)\, d\rho(y)\,, \tag{96}$$

where the square bracket means that the Lagrangian is computed as a function of the kernel of the fermionic projector $P_{\mathfrak{a},\mathfrak{b}}(x,y)$ (just as explained after (12) for the kernel $P(x,y)$). The identities (95) and (96) give a good intuitive understanding of how the action depends on the unitary operators $V_\mathfrak{a}$. We first note that in the case $\mathfrak{a} = \mathfrak{b}$, the unitary operators in (95) drop out, so that $P_{\mathfrak{a},\mathfrak{a}}(x,y) = P(x,y)$. This also explains why the first summand in (96) involves the original action $\mathcal{S}(\rho)$. In the $\mathfrak{a} \neq \mathfrak{b}$, however, the unitary operators in (95) do not drop out. In particular,

this makes it possible to introduce phase factors into the fermionic projector. For example, one may change the phase of each physical wave function $\psi^u_{\mathfrak{a}}$ arbitrarily while keeping the physical wave functions $\psi^u_{\mathfrak{b}}$ for $\mathfrak{b} \neq \mathfrak{a}$ unchanged. Choosing the resulting phases randomly, one gets destructive interference, implying that the kernel $P_{\mathfrak{a},\mathfrak{b}}(x, y)$ becomes small. Making use of this *dephasing effect*, one can make the summands in (96) for $\mathfrak{a} \neq \mathfrak{b}$ small. A detailed analysis of the involved scalings reveals that this indeed makes it possible to decrease the causal action (see [13]).

In words, this result means that minimizing the causal action triggers a mechanism which tends to decompose space-time M into many small sub-space-times $M_1, \ldots, M_L$. The physical wave functions in the different sub-space-times involve relative phases, with the effect that the correlations between the sub-space-times (as described by the kernels $P_{\mathfrak{a},\mathfrak{b}}(x, y)$) become small. Since the dephasing takes place on a microscopic length scale, this effect is referred to as *microscopic mixing*.

Let us discuss what microscopic mixing implies for the effective macroscopic interaction. One must distinguish two situations. One limiting case is complete dephasing, in which case $P_{\mathfrak{a},\mathfrak{b}}$ is approximately zero. As a result, there are no relations or structures between the two sub-space-times (note that for example the causal structure is encoded in the kernel of the fermionic projector; see Sect. 1.3). This entails that the two sub-space-times do not interact with each other. The resulting picture is that space-time looks effectively like a "superposition" of the different sub-space-times. This scenario is referred to as the *microscopic mixing of space-time regions*. The dephasing can be understood similar to decoherence effects in standard quantum field theory (see for example [31]).

If each of the microscopically mixed sub-space-times involves a different classical bosonic field, one obtains effectively a superposition of classical field configurations. This makes it possible to describe second-quantized bosonic fields (see [11]). However, as the different sub-space-times do not interact with each other, each sub-space-time has it own independent dynamics. This dynamics is described by the classical bosonic field in the corresponding sub-space-time.

In order to obtain an interaction via second-quantized bosonic fields, one needs to consider another limiting case in which the dephasing involves only some of the physical wave functions. In this case, the fermionic projector $P_{\mathfrak{a},\mathfrak{b}}$ is not necessarily small. This also implies that relations arising as a consequence of the collective behavior of all physical wave functions (like the causal relations or classical bosonic fields) still exist between the sub-space-times $M_{\mathfrak{a}}$ and $M_{\mathfrak{b}}$. In more physical terms, the sub-space-times still interact with each other. This scenario is studied in [13] and is referred to as the *microscopic mixing of wave functions*. In order to describe the effective interaction, one describes the unitary operators $V_{\mathfrak{a}}$ by random matrices. Taking averages over the random matrices, one finds that the effective interaction can be described perturbatively in terms of Feynman diagrams which involve both fermionic and bosonic loops. The appearance of bosonic loops can be understood by working with second-quantized bosonic fields. Working out the detailed combinatorics and the implications of the resulting quantum field theory is work in progress (for the first step in this program see [27]).

Acknowledgements I would like to thank the referee for helpful comments on the manuscript.

References

1. Y. Bernard, F. Finster, On the structure of minimizers of causal variational principles in the non-compact and equivariant settings. Adv. Calc. Var. **7**(1), 27–57 (2014). arXiv:1205.0403 [math-ph]
2. J. Bognár, *Indefinite Inner Product Spaces* (Springer, New York, 1974). Ergebnisse der Mathematik und ihrer Grenzgebiete, Band 78
3. L. Bombelli, J. Lee, D. Meyer, R.D. Sorkin, Space-time as a causal set. Phys. Rev. Lett. **59**(5), 521–524 (1987)
4. R. Brunetti, M. Dütsch, K. Fredenhagen, Perturbative algebraic quantum field theory and the renormalization groups. Adv. Theor. Math. Phys. **13**(5), 1541–1599 (2009). arXiv:0901.2038 [math-ph]
5. J. Dieudonné, *Foundations of Modern Analysis*. Enlarged and Corrected Printing, Pure and Applied Mathematics, vol. 10-I (Academic, New York/London, 1969)
6. F. Finster, *The Continuum Limit of Causal Fermion Systems* (in preparation). Book based on the preprints arXiv:0908.1542 [math-ph]; arXiv:1211.3351 [math-ph]; arXiv:1409.2568 [math-ph]
7. F. Finster, Definition of the dirac sea in the presence of external fields. Adv. Theor. Math. Phys. **2**(5), 963–985 (1998). arXiv:hep-th/9705006
8. F. Finster, *The Principle of the Fermionic Projector*. AMS/IP Studies in Advanced Mathematics, vol. 35 (American Mathematical Society, Providence, 2006). hep-th/0001048; hep-th/0202059; hep-th/0210121
9. F. Finster, A variational principle in discrete space-time: existence of minimizers. Calc. Var. Partial Differ. Eqns. **29**(4), 431–453 (2007). arXiv:math-ph/0503069
10. F. Finster, Causal variational principles on measure spaces. J. Reine Angew. Math. **646**, 141–194 (2010). arXiv:0811.2666 [math-ph]
11. F. Finster, Entanglement and second quantization in the framework of the fermionic projector. J. Phys. A Math. Theor. **43**, 395302 (2010). arXiv:0911.0076 [math-ph]
12. F. Finster, *The Chiral Index of the Fermionic Signature Operator* (2014). arXiv:1404.6625 [math-ph]
13. F. Finster, Perturbative quantum field theory in the framework of the fermionic projector. J. Math. Phys. **55**(4), 042301 (2014). arXiv:1310.4121 [math-ph]
14. F. Finster, A Lorentzian quantum geometry. Adv. Theor. Math. Phys. **16**(4), 1197–1290 (2012). arXiv:1107.2026 [math-ph]
15. F. Finster, On the initial value problem for causal variational principles. J. Reine Angew. Math. (2016, to appear). arXiv:1303.2964 [math-ph]
16. F. Finster, A. Grotz, The causal perturbation expansion revisited: rescaling the interacting Dirac sea. J. Math. Phys. **51**, 072301 (2010). arXiv:0901.0334 [math-ph]
17. F. Finster, A. Grotz, D. Schiefeneder, Causal fermion systems: a quantum space-time emerging from an action principle, in *Quantum Field Theory and Gravity*, ed. by F. Finster, O. Müller, M. Nardmann, J. Tolksdorf, E. Zeidler (Birkhäuser, Basel, 2012), pp. 157–182. arXiv:1102.2585 [math-ph]
18. F. Finster, N. Kamran, *Spinors on Singular Spaces and the Topology of Causal Fermion Systems* (2014). arXiv:1403.7885 [math-ph]
19. F. Finster, J. Kleiner, *The Jet Bundle Dynamics of Causal Fermion Systems* (in preparation)
20. F. Finster, J. Kleiner, *Noether-Like Theorems for Causal Variational Principles* (2015). arXiv:1506.09076 [math-ph]
21. F. Finster, J. Kleiner, *Causal Fermion Systems as a Candidate for a Unified Physical Theory* (2015). arXiv:1502.03587 [math-ph]

22. F. Finster, O. Müller, *Lorentzian Spectral Geometry for Globally Hyperbolic Surfaces* (2014). arXiv:1411.3578 [math-ph]
23. F. Finster, S. Murro, C. Röken, *The Fermionic Projector in a Time-Dependent External Potential: Mass Oscillation Property and Hadamard States*. arXiv:1501.05522 [math-ph]
24. F. Finster, M. Reintjes, *A Non-perturbative Construction of the Fermionic Projector on Globally Hyperbolic Manifolds II – Space-Times of Infinite Lifetime* (2013). arXiv:1312.7209 [math-ph]
25. F. Finster, M. Reintjes, A non-perturbative construction of the fermionic projector on globally hyperbolic manifolds I – space-times of finite lifetime. Adv. Theor. Math. Phys. (2015, to appear). arXiv:1301.5420 [math-ph]
26. F. Finster, D. Schiefeneder, On the support of minimizers of causal variational principles. Arch. Ration. Mech. Anal. **210**(2), 321–364 (2013). arXiv:1012.1589 [math-ph]
27. F. Finster, J. Tolksdorf, A microscopic derivation of quantum electrodynamics (in preparation)
28. F. Finster, J. Tolksdorf, Perturbative description of the fermionic projector: normalization, causality and Furry's theorem. J. Math. Phys. **55**(5), 052301 (2014). arXiv:1401.4353 [math-ph]
29. I.S. Gradshteyn, I.M. Ryzhik, *Table of Integrals, Series, and Products*, ed. by Ju. V. Geronimus, M. Ju. Ceuıtlin, 4th edn. (Academic, New York, 1965)
30. P.R. Halmos, *Measure Theory* (Springer, New York, 1974)
31. E. Joos, H.D. Zeh, C. Kiefer, D. Giulini, J. Kupsch, I.-O. Stamatescu, *Decoherence and the Appearance of a Classical World in Quantum Theory*, 2nd edn. (Springer, Berlin, 2003)
32. H. Langer, Spectral functions of definitizable operators in Krein spaces, in *Functional Analysis 1981*, Dubrovnik. Lecture Notes in Mathematics, vol. 948 (Springer, Berlin, 1982), pp. 1–46
33. P.D. Lax, *Functional Analysis*. Pure and Applied Mathematics (Wiley-Interscience, New York, 2002)
34. F.W.J. Olver, D.W. Lozier, R.F. Boisvert, C.W. Clark (eds.), *Digital Library of Mathematical Functions* (National Institute of Standards and Technology, Washington, DC, 2010). Release date 01/07/2011. From http://dlmf.nist.gov/
35. W. Rudin, *Principles of Mathematical Analysis*, International Series in Pure and Applied Mathematics, 3rd edn. (McGraw-Hill Book, New York/Auckland/Düsseldorf, 1976)

A Perspective on External Field QED

Dirk-André Deckert and Franz Merkl

Contents

Abstract In light of the conference *Quantum Mathematical Physics* held in Regensburg in 2014, we give our perspective on the external field problem in quantum electrodynamics (QED), i.e., QED without photons in which the sole interaction stems from an external, time-dependent, four-vector potential. Among others, this model was considered by Dirac, Schwinger, Feynman, and Dyson as a model to describe the phenomenon of electron-positron pair creation in regimes in which the interaction between electrons can be neglected and a mean field description of the photon degrees of freedom is valid (e.g., static field of heavy nuclei or lasers fields). Although it may appear as second easiest model to study, it already bares a severe divergence in its equations of motion preventing any straight-forward construction of the corresponding evolution operator. In informal computations of the vacuum polarization current this divergence leads to the need of the so-called *charge renormalization*. In an attempt to provide a bridge between physics and mathematics, this work gives a review ranging from the heuristic picture to our rigorous results in a way that is hopefully also accessible to non-experts and students. We discuss how the evolution operator can be constructed, how this

D. Deckert (✉) • F. Merkl
Mathematisches Institut, Ludwig-Maximilians-Universität München, Theresienstr. 39, 80333 München, Germany
e-mail: deckert@math.lmu.de; merkl@math.lmu.de

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_16

construction yields well-defined and unique transition probabilities, and how it provides a family of candidates for charge current operators without the need of removing ill-defined quantities. We conclude with an outlook of what needs to be done to identify the physical charge current among this family.

Keywords Quantum electrodynamics • External field • Evolution operator • Polarization classes • Geometric phase • Charge current • Vacuum polarization

Mathematics Subject Classification (2010). Primary: 81V10; Secondary: 81T08, 46N50

1 Heuristic Introduction

We begin with a basic and informal introduction inspired by Dirac's original work [9] to provide a physical intuition for the external field QED model. Specialists among the readers are referred directly to Sect. 1.1. As it is well-known, the free one-particle Dirac equation, in units such that $\hbar = 1$ and $c = 1$,

$$(i\partial\!\!\!/ - m)\psi(x) = 0, \qquad \text{for } \psi \in \mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4), \tag{1}$$

was originally suggested to describe free motion of single electrons. Curiously enough, it allows for wave functions in the negative part $(-\infty, -m]$ of the energy spectrum $\sigma(H^0) = (-\infty, -m] \cap [+m, \infty)$ of the corresponding Hamiltonian $H^0 = \gamma^0(-i\boldsymbol{\gamma} \cdot \nabla + m)$. As the spectrum is not bounded from below, physicists rightfully argue [17] that a Dirac electron coupled to the electromagnetic field may cascade to ever lower and lower energies by means of radiation; the reason for this unphysical instability is that the electromagnetic field is an open system, which may transport energy to spacial infinity. Other peculiarities stemming from the presence of a negative energy spectrum are the so-called *Zitterbewegung* first observed by Schrödinger [29] and *Klein's paradox* [20]. As Dirac demonstrated [9], those peculiarities can be reconciled in a coherent description when switching from the one-particle Dirac equation (1) to a many, in the mathematical idealization even infinitely many, particle description known as the *second-quantization* of the Dirac equation. Perhaps the most striking consequence of this description is the phenomenon of electron-positron pair creation, which only little later was observed experimentally by Anderson [1].

In order to get rid of peculiarities due to the negative energy states, Dirac proposed to introduce a "sea" of electrons occupying all negative energy states. The Pauli exclusion principle then acts to prevent any additional electron in the positive part of the spectrum to dive into the negative one. Let us introduce the orthogonal projectors P^+ and P^- onto the positive and negative energy subspaces $\mathcal{H}^+$ and $\mathcal{H}^-$, respectively, i.e., $\mathcal{H}^+ = P^+\mathcal{H}$ and $\mathcal{H}^- = P^-\mathcal{H}$. Dirac's heuristic picture amounts

to introducing an infinitely many-particle wave function of this sea of electrons, usually referred to as *Dirac sea*,

$$\Omega = \varphi_1 \wedge \varphi_2 \wedge \varphi_3 \wedge \ldots, \qquad (\varphi_n)_{n\in\mathbb{N}} \text{ being an orthonormal basis of } \mathcal{H}^-, \tag{2}$$

where $\wedge$ denotes the antisymmetric tensor product w.r.t. Hilbert space $\mathcal{H}$. Given a one-particle evolution operator $U : \mathcal{H} \circlearrowleft$, such a Dirac sea may then be evolved with an operator $\mathcal{L}_U$ according to

$$\mathcal{L}_U\Omega = U\varphi_1 \wedge U\varphi_2 \wedge U\varphi_3 \wedge \ldots. \tag{3}$$

Such an ansatz may seem academic and ad-hoc. First, the Coulomb repulsion between the electrons is neglected (not to mention radiation), second, the choice of Ω is somewhat arbitrary. These assumptions clearly would have to be justified starting from a yet to be found full version of QED. For the time being we can only trust Dirac's intuition that the Dirac sea, when left alone, is so homogeneously distributed that effectively every electron in it feels the same net interaction from each solid angle, and in turn, moves freely so that it lies near to neglect the Coulomb repulsion; see also [3] for a more detailed discussion. Since then none of the particles effectively "sees" the others, physicists refer to such a state as the "vacuum". A less ad-hoc candidate for Ω would of course be the ground state of a fully interacting theory. Even though the net interaction may cancel out, electrons in the ground state will be highly entangled. The hope in using the product state (2) instead, i.e., the ground state of the free theory, to model the vacuum is that in certain regimes the particular entanglement and motion deep down in the sea might be irrelevant. The success of QED in arriving at predictions which are in astonishing agreement with experimental data substantiates this hope.

As a first step to introduce an interaction one allows for an external disturbance of the electrons in Ω modeled by a prescribed, time-dependent, four-vector potential A. This turns the one-particle Dirac equation into

$$(i\partial\!\!\!/ - m)\psi(x) = eA\!\!\!/(x)\psi(x). \tag{4}$$

The potential A may now allow for transitions of states between the subspaces $\mathcal{H}^+$ and $\mathcal{H}^-$. Heuristically speaking, a state $\varphi_1 \in \mathcal{H}$ in the Dirac sea Ω may be bound by the potential and over time dragged to the positive energy subspace $\chi \in \mathcal{H}^+$. For an (as we shall see, oversimplified) example, let us assume that up to a phase the resulting state can be represented as

$$\Psi = \chi \wedge \varphi_2 \wedge \varphi_3 \wedge \ldots \tag{5}$$

in which φ_1 is missing. Due to (4), states in $\mathcal{H}^+$ move rather differently as compared to the ones in $\mathcal{H}^-$. Thus, an electron described by $\chi \in \mathcal{H}^+$ will emerge from the "vacuum" and so does the "hole" described by the missing $\varphi_1 \in \mathcal{H}^-$ in the Dirac sea (5), which is left behind. Following Dirac, the *hole* itself can be interpreted as a

particle, which is referred to as *positron*, and both names can be used as synonyms. If, as in this example, the electrons deeper down in the sea are not affected too much by this disturbance, it makes sense to switch to a more economic description. Instead of tracking all infinitely many particles, it then suffices to describe the motion of the electron χ, of the corresponding hole φ_1, and of the net evolution of Ω only. Since the number of electron-hole pairs may vary over time, a formalism for variable particle numbers is needed. This is provided by the Fock space formalism of quantum field theory, i.e., the so-called "second quantization". One introduces a so-called *creation* operator a^* that formally acts as

$$a^*(\chi)\varphi_1 \wedge \varphi_2 \wedge \ldots = \chi \wedge \varphi_1 \wedge \varphi_2 \wedge \ldots, \tag{6}$$

and also its corresponding adjoint a, which is called *annihilation* operator. The state Ψ from example in (5) can then be written as $\Psi = a^*(\chi)a(\varphi_1)\Omega$. With the help of a^*, one-particle operators like the evolution operator U^A generated by (4) can be lifted to an operator $\tilde{U}$ on $\mathcal{F}$ in a canonical way by requiring that

$$\tilde{U}^A a^*(f)(\tilde{U}^A)^{-1} = a^*(U^A f). \tag{7}$$

This condition determines a lift up to a phase as can be seen from the left-hand side of (7). Since the operator $a^*(f)$ is linear in its argument $f \in \mathcal{H}$, it is commonly split into the sum

$$a^*(f) = b^*(f) + c^*(f) \qquad \text{with} \qquad b^*(f) := a^*(P^+ f), \quad c^*(f) := a^*(P^- f). \tag{8}$$

Hence, b^* and c^* and their adjoints are creation and annihilation operators of electrons having positive and negative energy, respectively. In order to be able to disregard the infinitely many-particle wave function Ω in the notation, one introduces the following change in language. First, the space generated by states of the form $b^*(f_1)b^*(f_2)\ldots b^*(f_n)\Omega$ for $f_k \in \mathcal{H}^+$ is identified with the *electron Fock space*

$$\mathcal{F}_e = \bigoplus_{n\in\mathbb{N}_0} (\mathcal{H}^+)^{\wedge n}. \tag{9}$$

Second, the space generated by the states of the form $c(g_1)c(g_2)\ldots c(g_n)\Omega$ for $g_k \in \mathcal{H}^-$ is identified with the *hole Fock space*

$$\mathcal{F}_h = \bigoplus_{n\in\mathbb{N}_0} (\mathcal{H}^-)^{\wedge n}. \tag{10}$$

Note that this time the *annihilation* operator of *negative* energy states is employed to generate the Fock space. To make this evident in the notation, one usually replaces

$c(g)$ by a creation operator $d^*(g)$. However, unlike creation operators, $c(g)$ is *anti-linear* in its argument $g \in \mathcal{H}^-$. Thus, in a third step one replaces $\mathcal{H}^-$ by its complex conjugate $\overline{\mathcal{H}^-}$, i.e., the set $\mathcal{H}^-$ equipped with the usual $\mathbb{C}$-vector space structure except for the scalar multiplication $\cdot^\star : \mathbb{C} \times \overline{\mathcal{H}^-} \to \overline{\mathcal{H}^-}$ which is redefined by $\lambda \cdot^\star g = \lambda^* g$ for all $\lambda \in \mathbb{C}$ and $g \in \overline{\mathcal{H}^-}$. This turns $\mathcal{F}_h$ into

$$\overline{\mathcal{F}_h} = \bigoplus_{n\in\mathbb{N}_0} (\overline{\mathcal{H}^-})^{\wedge n}, \tag{11}$$

and the hole creation operator $d^*(g) = c(g)$ becomes *linear* in its argument $g \in \overline{\mathcal{H}^-}$. To treat electrons and holes more symmetrically, one also introduces the *anti-linear* charge conjugation operator $C : \mathcal{H} \to \mathcal{H}$, $C\psi = i\gamma^2\psi^*$. This operator exchanges $\mathcal{H}^+$ and $\mathcal{H}^-$, i.e., $C\mathcal{H}^\pm = \mathcal{H}^\mp$, and thus, gives rise to a *linear* map $C : \overline{\mathcal{H}^-} \to \mathcal{H}^+$. A hole wave function $g \in \overline{\mathcal{H}^-}$ living in the space negative states can then be represented by a wave function $Cg \in \mathcal{H}^+$ living in the positive energy space. Our discussion of the Dirac sea above may appear to break the charge symmetry as Ω is represented by a sea of electrons in $\mathcal{H}^-$. However, an equivalent description that makes the charge symmetry explicit is possible by representing the vacuum Ω through a pair of two seas, one in $\mathcal{H}^+$ and one in $\mathcal{H}^-$. Nevertheless, as the charge symmetry will not play a role in this overview we will continue using Dirac's picture with a sea of electrons in $\mathcal{H}^-$.

By definition (6) it can be seen that b, b^* and d, d^* fulfill the well-known anti-commutator relations:

$$\begin{aligned} \{b(g), b(h)\} &= 0 = \{b^*(g), b^*(h)\}, & \{b^*(g), b(h)\} &= \langle g, P^+ h\rangle \,\mathrm{id}_{\mathcal{F}_e}, \\ \{d(g), d(h)\} &= 0 = \{d^*(g), d^*(h)\}, & \{d^*(g), d(h)\} &= \langle g, P^- h\rangle \,\mathrm{id}_{\overline{\mathcal{F}_h}}. \end{aligned} \tag{12}$$

The full Fock space for the electrons and positrons is then given by

$$\mathcal{F} = \mathcal{F}_e \otimes \overline{\mathcal{F}_h}. \tag{13}$$

In this space the vacuum wave function Ω in (2) is represented by $|0\rangle = 1 \otimes 1$ and the pair state Ψ in (5) by $a^*(\chi)d^*(\varphi_1)|0\rangle$. Thus, in this notation one only describes the excitations of the vacuum, i.e., those electrons that deviate from it. The infinitely many other electrons in the Dirac sea one preferably would like to forget about are successfully hidden in the symbol $|0\rangle$. Here, however, the story ends abruptly.

1.1 The Problem and a Program for a Cure

For a prescribed external potential A, one would be inclined to compute transition probabilities for the creation of pairs, as for example for a transition from Ω to Ψ as in (2) and (5), right away. Given the one-particle Dirac evolution operator

$U^A = U^A(t_1, t_0)$ generated by (4) and any orthonormal basis $(\chi_n)_n$ of $\mathcal{H}^+$, the first order of perturbation of the probability of a possible pair creation is given by

$$\sum_{nm} \left|\langle \chi_n, U^A \varphi_m \rangle\right|^2 = \|U^A_{+-}\|_{I_2}, \tag{14}$$

where $I_2(\mathcal{H})$ denotes the space of bounded operators with finite Hilbert-Schmidt norm $\|\cdot\|_{I_2}$, and we use the notation $U^A_{\pm\mp} = P^{\pm} U^A P^{\mp}$. For quite general potentials $A = (A^0, \mathbf{A})$, it turns out that:

Theorem 1.1 ([26]) *Term* (14) $< \infty$ *for all times* $t_0, t_1 \in \mathbb{R} \Leftrightarrow \boldsymbol{A} = 0$.

In view of (14), the transition probability is thus only defined for external potentials A that have zero spatial components $\mathbf{A}$. Even worse, the criterion for the well-definedness of a possible lift $\tilde{U}$ of any unitary one-particle operator U according to (7) is given by:

Theorem 1.2 ([30]) *There is a unitary operator* $\tilde{U} : \mathcal{F} \circlearrowleft$ *that fulfills* (7) $\Leftrightarrow$ $U_{+-}, U_{-+} \in I_2(\mathcal{H})$.

Applying this result to the evolution operator U^A, (14) and Theorem 1.1 imply that the criterion in Theorem 1.2 is only fulfilled for external potentials A with zero spatial components $\mathbf{A}$. Even more peculiar, the given criterion is not gauge covariant (not to mention the Lorentz covariance). Although the free evolution operator $U^{A=0}$ has a lift, in the case that some spatial derivatives of a scalar field Γ are non-zero, the gauge transformed $U^{A=\partial\Gamma}$ does not. This indicates that an unphysical assumption must have been made.

What singles out the spatial components of A? Mathematically, they appear in the Hamiltonian, $H^A = \gamma^0(-i\boldsymbol{\gamma}\cdot\boldsymbol{\Delta} + m) + A_0 - \gamma^0\boldsymbol{\gamma}\cdot\mathbf{A}$, preceded by the spinor matrix $\gamma^0\boldsymbol{\gamma}$ whereas A_0 is only a multiple of the identity. Heuristically, if $\mathbf{A}$ is non-zero then the $\gamma^0\boldsymbol{\gamma}$ matrix transforms the negative energy states φ_n in spinor space to develop components in $\mathcal{H}^+$. There is no mechanism that would limit this development, not even smallness of $|\mathbf{A}|$, so there is no reason why the infinite sum (14) should be finite – and in general this is also not the case as Theorem 1.1 shows. In other words, for $\mathbf{A} \neq 0$, instantly infinitely many electron-positron pairs are created from the vacuum state Ω. Therefore, the picture is not nearly as peaceful as suggested by example state (5). However, if A is switched off at some later time one can expect that almost all of these pairs disappear again, and only a few excitations of the vacuum as in (5) will remain (hence, the name *virtual pairs* that is used by physicists). Assuming that at initial and final times $A = 0$, it can indeed be shown that the scattering matrix S^A fulfills the conditions of Theorem 1.2. The physical reason why the spatial components are singled out is due to the use of equal-time hyperplanes and will be discussed more geometrically in Sect. 2; see Theorem 2.8 below.

In conclusion, the problem lies in the fact that even the "vacuum" Ω consists of infinitely many particles. In the formalism of the free theory this fact is usually hidden by the use of normal ordering. Without it the ground state energy of Ω would be the infinite sum of all negative energies, or the charge current operator

expectation value $\langle \Omega, \overline{a}\gamma^\mu a\Omega\rangle$ of the vacuum would simply be the infinite sum of all one-particle currents $\overline{\varphi}_n\gamma^\mu\varphi_n$ – both quantities that diverge. The rational behind the ad-hoc introduction of normal ordering of, e.g., the charge current operator is again the assumption that in the vacuum state these currents are effectively not observable since the net interaction between the particles vanishes.

The incompatibility of Theorem 1.2 with the gauge freedom however shows that, although the choice of Ω may be distinguished for $A = 0$ by the ground state property, it is somehow arbitrary when $A \neq 0$, and so is the choice in the splitting of $\mathcal{H}$ into $\mathcal{H}^+$ and $\mathcal{H}^-$, which is usually referred to as *polarization*. As a program for a cure of these divergences, one may therefore attempt to carefully adapt the choice of the polarization depending on the evolution of A instead of keeping it fixed. Several attempts have been made to give a definition of a more physical polarization, one of them being the *Furry picture*. It defines the polarization according to the positive and negative parts of the spectrum of H^A given a fixed A. Unfortunately, none of the proposed choices are Lorentz invariant as it is shown in [10] since the vacuum state w.r.t. one of such choices in one frame of reference may appear as a many-particle state in another. This is due to the fact that the energy spectrum is obviously not invariant under Lorentz boosts.

Although a fully developed QED may be able to distinguish a class of states that can be regarded as physical vacuum states, simply by verifying the assumption above that the net interaction between the particles vanishes, the external field QED model has no mathematical structure to do so. Nevertheless, whenever a distinction between electrons and positrons by means of a polarization is not necessary, e.g., in the case of vacuum polarization in which the exact number of pairs is irrelevant, it should still be possible to track the time evolution $\tilde{U}^A\Omega$ and study the generated dynamics – not only asymptotically in scattering theory but also at intermediate times. The choice in admissible polarizations can then be seen to be analogous to the choice of a convenient coordinate system to represent the Dirac seas. Since the employed Fock space $\mathcal{F}$ depends directly on the polarization of $\mathcal{H}$ into $\mathcal{H}^+$ and $\mathcal{H}^-$, see (9)–(10) and (13), the standard formalism has to be adapted to allow the Fock space to also vary according to A, and the evolution operator $\tilde{U}^A$ must be implemented mapping one Fock space into another. While the idea of varying Fock space may be unfamiliar from the non-relativistic setting, it is natural when considering a relativistic formalism. A Lorentz boost, for example, tilts an equal-time hyperplane to a Cauchy surface Σ which requires a change from the standard Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$ to one that is attached to Σ, and likewise, for the corresponding Fock spaces. Hence, a Lorentz transform will naturally be described by a map from one Fock space into another [5]. In the special case of equal-time hyperplanes, parts of this program have been carried out in [21, 22] and [4]. In the former two works the time evolution operator is nevertheless implemented on standard Fock space $\mathcal{F}$ by conjugation of the evolution operator with a convenient (non-unique) unitary "renormalization" transformation. In the latter work it is implemented between time-varying Fock spaces, so-called infinite wedge spaces, and furthermore, the degrees of freedom in the construction have been identified. These latter results have been extended recently to allow for general

Cauchy surfaces in [5, 6] and are presented in Sect. 2. All these results ensure the existence of an evolution operator by a quite abstract argument. Therefore, we review a construction of it in Sect. 3 based on [4]. It utilizes a notation that is very close to Dirac's original view of a sea of electrons as in (2). Though it is canonically equivalent to the Fock space formalism, it provided us a more intuitive view of the problem and helped in identifying the degrees of freedom involved in the construction. In Sect. 4 we conclude with a discussion of the unidentified phase of the evolution operator and its meaning for the charge current in. Beside the publications cited so far, there are several recent contributions which also take up on Dirac's original idea. As a more fundamental approach we want to mention the one of the so-called "Theory of Causal Fermion Systems" [11–13], which is based on a reformulation of quantum electrodynamics from first principles. The phenomenon of adiabatic pair creation was treated rigorously in [24]. Furthermore, there is a series of works treating the Dirac sea in the Hartree-Fock approximation. The most general is [16] in which the effect of vacuum polarization was treated self-consistently for static external sources.

2 Varying Fock Spaces

In order to better understand why the spatial components of A had been singled out in the discussion above, it is helpful to consider the Dirac evolution not only on equal-time hyperplanes but on more general Cauchy surfaces.

Definition 2.1 A Cauchy surface Σ in $\mathbb{R}^4$ is a smooth, 3-dimensional submanifold of $\mathbb{R}^4$ that fulfills the following two conditions:

(a) Every inextensible, two-sided, time- or light-like, continuous path in $\mathbb{R}^4$ intersects Σ in a unique point.
(b) For every $x \in \Sigma$, the tangent space $T_x\Sigma$ of Σ at x is space-like.

To each Cauchy surface Σ we associated a Hilbert space $\mathcal{H}_\Sigma$.

Definition 2.2 Let $\mathcal{H}_\Sigma = L^2(\Sigma, \mathbb{C}^4)$ denote the vector space of all 4-spinor valued measurable functions $\phi : \Sigma \to \mathbb{C}^4$ (modulo changes on null sets) having a finite norm $\|\phi\| = \sqrt{\langle \phi, \phi \rangle} < \infty$ w.r.t. the scalar product

$$\langle \phi, \psi \rangle = \int_\Sigma \overline{\phi(x)} i_\gamma(d^4x) \psi(x). \tag{15}$$

Here, $i_\gamma(d^4x)$ denotes the contraction of the volume form $d^4x = dx^0 \wedge dx^1 \wedge dx^2 \wedge dx^3$ with the spinor-matrix valued vector γ^μ, $\mu = 0, 1, 2, 3$. The corresponding dense subset of smooth and compactly supported functions will be denoted by $\mathcal{C}_\Sigma$.

The well-posedness of the initial value problem related to (4) for initial data on Cauchy surfaces has been studied in the literature; e.g., see [18, 31] for

general hyperbolic systems and more specifically for wave equations on Lorentzian manifolds [2, 8, 14, 25], and [7]. For the purpose of our study we furthermore introduced generalized Fourier transforms for the Dirac equation in [5] and extended the standard Sobolev and Paley-Wiener methods in $\mathbb{R}^n$ to the geometry given by the Cauchy surfaces and the mass shell of the Dirac equation. These methods were required for the analysis of solutions. They play along nicely with Lorentz and gauge transforms and allow for the introduction of an interaction picture. As a byproduct, these methods also ensure existence, uniqueness, and causal structure of strong solutions. Since we avoid technicalities in this paper, we assume A is a smooth and compactly supported (although sufficient strong decay would be sufficient), and the following theorem will suffice to discuss the one-particle Dirac evolution.

Theorem 2.3 (Theorem 2.23 in [5]) *Let Σ, Σ' be two Cauchy surfaces and $\psi_\Sigma \in \mathcal{C}_\Sigma$ the initial data. There is a unique strong solution $\psi \in \mathcal{C}^\infty(\mathbb{R}^4, \mathbb{C}^4)$ to (4) being supported in the forward and backward light cone of* $\operatorname{supp}\psi_\Sigma$ *such that $\psi|_\Sigma = \psi_\Sigma$ holds. Furthermore, there is an isometric isomorphism $U^A_{\Sigma'\Sigma} : \mathcal{C}_\Sigma \to \mathcal{C}_{\Sigma'}$ fulfilling $\psi|_{\Sigma'} = U^A_{\Sigma'\Sigma}\psi_\Sigma$. Its unique extension to a unitary map $U^A_{\Sigma'\Sigma} : \mathcal{H}_\Sigma \to \mathcal{H}_{\Sigma'}$ is denoted by the same symbol.*

Similarly to the standard Fock space (13) we define the Fock space for a Cauchy surface on the basis of a polarization.

Definition 2.4 Let $\mathtt{Pol}(\mathcal{H}_\Sigma)$ denote the set of all closed, linear subspaces $V \subset \mathcal{H}_\Sigma$ such that V and $V^\perp$ are both infinite dimensional. Any $V \in \mathtt{Pol}(\mathcal{H}_\Sigma)$ is called a *polarization* of $\mathcal{H}_\Sigma$. For $V \in \mathtt{Pol}(\mathcal{H}_\Sigma)$, let $P^V_\Sigma : \mathcal{H}_\Sigma \to V$ denote the orthogonal projection of $\mathcal{H}_\Sigma$ onto V.

The Fock space attached to Cauchy surface Σ and corresponding to polarization $V \in \mathtt{Pol}(\mathcal{H}_\Sigma)$ is defined by

$$\mathcal{F}(V,\Sigma) := \bigoplus_{c\in\mathbb{Z}} \mathcal{F}_c(V,\mathcal{H}_\Sigma), \qquad \mathcal{F}_c(V,\Sigma) := \bigoplus_{\substack{n,m\in\mathbb{N}_0\\ c=m-n}} (V^\perp)^{\wedge n} \otimes \overline{V}^{\wedge m}. \tag{16}$$

Note that the standard Fock space is included in this definition by choosing $\Sigma = \{0\}\times\mathbb{R}^3$ and $V = \mathcal{H}^-$.

Given two Cauchy surfaces Σ and Σ', polarizations $V \in \mathtt{Pol}(\mathcal{H}_\Sigma)$ and $V' \in \mathtt{Pol}(\mathcal{H}_{\Sigma'})$, and the one-particle evolution operator $U^A_{\Sigma'\Sigma} : \mathcal{H}_\Sigma \to \mathcal{H}_{\Sigma'}$, we need a condition analogous to (7) that allows us to find an evolution operator $\tilde{U}^A_{V',\Sigma';V,\Sigma} : \mathcal{F}(V,\Sigma) \to \mathcal{F}(V',\Sigma')$. For the discussion, let a^*_Σ and a_Σ denote the corresponding creation and annihilation operators on any $\mathcal{F}(W,\Sigma)$ for $W \in \mathtt{Pol}(\mathcal{H}_\Sigma)$; note that the defining expression of a^* in (6) does not depend on the choice of a polarization W. In this notation, the lift requirement reads

$$\tilde{U}^A_{V',\Sigma';V,\Sigma}\, a^*_\Sigma(f)\, \big(\tilde{U}^A_{V',\Sigma';V,\Sigma}\big)^{-1} = a^*_{\Sigma'}(U^A_{\Sigma'\Sigma}f), \qquad \forall f \in \mathcal{H}_\Sigma. \tag{17}$$

The condition under which such a lift of the one-particle evolution operator $U^A_{\Sigma'\Sigma}$ exists can be inferred from a slightly rewritten version of the Shale-Stinespring Theorem 1.2:

Corollary 2.5 *Let Σ, Σ' be Cauchy surfaces, $V \in \mathtt{Pol}(\mathcal{H}_\Sigma)$, and $V' \in \mathtt{Pol}(\mathcal{H}_{\Sigma'})$. Then the following statements are equivalent:*

(a) There is a unitary operator $\tilde{U}^A_{V'\Sigma';V,\Sigma} : \mathcal{F}(V,\Sigma) \to \mathcal{F}(V',\Sigma')$ which fulfills (17).

(b) The off-diagonals $P^{V'^\perp}_{\Sigma'} U^A_{\Sigma'\Sigma} P^V_\Sigma$ and $P^{V'}_{\Sigma'} U^A_{\Sigma'\Sigma} P^{V^\perp}_\Sigma$ are Hilbert-Schmidt operators.

Note again that if such a lift exists, its phase is not fixed by (17) and the corollary above does not provide any information about it. Therefore, we will discuss a direct construction of the lifted operator $\tilde{U}^A_{V'\Sigma';V,\Sigma}$ in Sect. 3, which makes the involved degrees of freedom apparent.

Coming back to the question which polarizations $V \in \mathtt{Pol}(\mathcal{H}_\Sigma)$ and $V' \in \mathtt{Pol}(\mathcal{H}_{\Sigma'})$ guarantee the existence of a lifted evolution operator $\tilde{U}^A_{\Sigma'\Sigma} : \mathcal{F}(V,\Sigma) \to \mathcal{F}(V',\Sigma')$, one readily finds a trivial choice. Let us pick a Cauchy surface Σ_{in} in the remote past fulfilling:

$$\Sigma_{\mathrm{in}} \text{ is a Cauchy surface such that } \operatorname{supp} A \cap \Sigma_{\mathrm{in}} = \emptyset. \tag{18}$$

When transporting the standard polarization along with the Dirac evolution we get

$$V = U^A_{\Sigma\Sigma_{\mathrm{in}}} P^-_{\Sigma_{\mathrm{in}}} \mathcal{H}_{\Sigma_{\mathrm{in}}} \in \mathtt{Pol}(\mathcal{H}_\Sigma), \qquad V' = U^A_{\Sigma'\Sigma_{\mathrm{in}}} P^-_{\Sigma_{\mathrm{in}}} \mathcal{H}_{\Sigma_{\mathrm{in}}} \in \mathtt{Pol}(\mathcal{H}_{\Sigma'}), \tag{19}$$

which automatically fulfills condition (b) of Theorem 2.5 as then the off-diagonals $(U^A_{\Sigma\Sigma_{\mathrm{in}}})_{\pm\mp}$ become zero. This choice is usually called the *interpolation picture*. Its drawback is that the polarizations V and V' depend on the whole history of A between Σ_{in} and Σ and Σ'. Moreover, such V and V' are rather implicit. Luckily, there are other choices. Statement (b) in Theorem 2.5 allows to differ from the projectors P^V_Σ and $P^{V'}_{\Sigma'}$ by a Hilbert-Schmidt operator. Hence, all admissible polarizations can be collected and characterized by means of the following classes:

Definition 2.6 For a Cauchy surface Σ we define the class

$$\mathtt{C}_\Sigma(A) := \left\{ W \in \mathtt{Pol}(\mathcal{H}_\Sigma) \,\middle|\, W \approx U^A_{\Sigma\Sigma_{\mathrm{in}}} \mathcal{H}^-_{\Sigma_{\mathrm{in}}} \right\} \tag{20}$$

where for $V, W \in \mathtt{Pol}(\mathcal{H}_\Sigma)$, $V \approx W$ means that the difference of the corresponding orthogonal projectors $P^V_\Sigma - P^W_\Sigma$ is a Hilbert-Schmidt operator.

As simple implication of Corollary 2.5 one gets:

Corollary 2.7 *Let Σ, Σ' be Cauchy surfaces and polarizations $V \in C_\Sigma(A)$ and $W \in C_{\Sigma'}(A)$. Then up to a phase there is a unitary operator $\tilde{U}^A_{\Sigma'\Sigma} : \mathcal{F}(V, \mathcal{H}_\Sigma) \to \mathcal{F}(W, \mathcal{H}_{\Sigma'})$ obeying (17).*

We emphasize again that any other possible polarization than the choice in (19) is comprised in the respective class $C_\Sigma(A)$ as Corollary 2.5 only allows for the freedom encoded in the equivalence relation $\approx$. Although the polarization (19) depends on the history of the evolution it turns out that the classes $C_\Sigma(A)$ are independent thereof. The sole dependence of the classes $C_\Sigma(A)$ is on the tangential components of A, which can be stated as follows.

Theorem 2.8 (Theorem 1.5 in [6]) *Let Σ be a Cauchy surface and let A and $\tilde{A}$ be two smooth and compactly supported external fields. Then*

$$C_\Sigma(A) = C_\Sigma(\tilde{A}) \qquad \Leftrightarrow \qquad A|_{T\Sigma} = \tilde{A}|_{T\Sigma}, \tag{21}$$

where $A|_{T\Sigma} = \tilde{A}|_{T\Sigma}$ means that for all x in Σ and all vectors y in the tangent space $T_x\Sigma$ of Σ at x, the relation $A_\mu(x)y^\mu = \tilde{A}_\mu(x)y^\mu$ holds.

This theorem is a generalization of Ruijsenaar's result [27] and helps to understand why on equal-time hyperplanes the spatial components of A appeared to play such a special role. The spatial components $\mathbf{A}$ are the tangential ones w.r.t. such Cauchy surfaces. Furthermore, the classes $C_\Sigma(A)$ transform nicely under Lorentz and gauge transformations:

Theorem 2.9 (Theorem 1.6 in [6])

(i) Consider a Lorentz transformation given by $L^{(S,\Lambda)}_\Sigma : \mathcal{H}_\Sigma \to \mathcal{H}_{\Lambda\Sigma}$ for a spinor transformation matrix $S \in \mathbb{C}^{4\times4}$ and an associated proper orthochronous Lorentz transformation matrix $\Lambda \in \mathrm{SO}^\uparrow(1,3)$, see for example [5, Section 2.3]. Then:

$$V \in C_\Sigma(A) \qquad \Leftrightarrow \qquad L^{(S,\Lambda)}_\Sigma V \in C_{\Lambda\Sigma}(\Lambda A(\Lambda^{-1}\cdot)). \tag{22}$$

(ii) Consider a gauge transformation $A' = A + \partial\Gamma$ for some $\Gamma \in C^\infty_c(\mathbb{R}^4, \mathbb{R})$ given by the multiplication operator $e^{-i\Gamma} : \mathcal{H}_\Sigma \to \mathcal{H}_\Sigma$, $\psi \mapsto \psi' = e^{-i\Gamma}\psi$. Then:

$$V \in C_\Sigma(A) \qquad \Leftrightarrow \qquad e^{-i\Gamma}V \in C_\Sigma(A + \partial\Gamma). \tag{23}$$

As an analogy from geometry one could think of the particular polarization as a particular choice of coordinates to represent the Dirac sea. Corollary 2.5 and Theorem 2.9 explain why gauge transformations that introduce spatial components in the external fields do not comply with the condition to the Shale-Stinespring Theorem 1.2 in which the "coordinates" $\mathcal{H}^+$ and $\mathcal{H}^-$ were fixed.

The key idea in the proofs of Theorems 2.8 and 2.9 is to guess a simple enough operator $P^A_\Sigma : \mathcal{H}_\Sigma \circlearrowleft$ depending only on the restriction $A|_\Sigma$ so that

$$U^A_{\Sigma\Sigma_{\mathrm{in}}} P^-_{\Sigma_{\mathrm{in}}} U^A_{\Sigma_{\mathrm{in}}\Sigma} - P^A_\Sigma \in I_2(\mathcal{H}_\Sigma), \qquad \text{and} \qquad (P^A_\Sigma)^2 - P^A_\Sigma \in I_2(\mathcal{H}_\Sigma). \tag{24}$$

The claims about the properties of the polarization classes $C_\Sigma(A)$ can then be inferred directly from the properties of P^A_Σ. This is due to the fact that (24) is compatible with the Hilbert-Schmidt operator freedom encoded in the $\approx$ equivalence relation. The intuition behind the guess of P^A_Σ used in the proofs presented in [6] comes from the gauge transform. Imagine the special situation in which an external potential A could be gauged to zero, i.e., $A = \partial\Gamma$ for a given scalar field Γ. In this case $e^{-i\Gamma}P^-_\Sigma e^{i\Gamma}$ is a good candidate for P^A_Σ. Now in the case of general external potentials A that cannot be attained by a gauge transformation of the zero potential, the idea is to implement gauge transforms locally at each space-time point. For example, if $p_-(x,y)$ denotes the informal integral kernel of the operator P^-_Σ, one could try to define P^A_Σ as the operator corresponding to the informal kernel $p^A(x,y) = e^{-i\lambda_A(x,y)}p_-(x,y)$ for the choice $\lambda_A(x) = A(x)_\mu(y-x)^\mu$. The effect of $\lambda_A(x,y)$ on the projector can be interpreted as a local gauge transform of $p_-(x,y)$ from the zero potential to the potential $A_\mu(x)$ at space-time point x. A careful analysis of P^A_Σ, which was conducted in Section 2 of [6], shows that P^A_Σ fulfills (24).

Finally, given Cauchy surface Σ, there is also an explicit representative of the polarization class $C_\Sigma(A)$ which can be given in terms of the bounded operator $Q^A_\Sigma : \mathcal{H}_\Sigma \circlearrowleft$ defined by

$$Q^A_\Sigma := P^+_\Sigma(P^A_\Sigma - P^-_\Sigma)P^-_\Sigma - P^-_\Sigma(P^A_\Sigma - P^-_\Sigma)P^+_\Sigma. \tag{25}$$

With it, the polarization class can be identified as follows:

Theorem 2.10 (Theorem 1.7 in [6]) *Given Cauchy surface* Σ*,*

$$C_\Sigma(A) = \left[e^{Q_\Sigma(A)}\mathcal{H}^-_\Sigma\right]_\approx .$$

The implications of these results on the physical picture can be seen as follows. The Dirac sea on Cauchy surface Σ can be described in any Fock space $\mathcal{F}(V,\mathcal{H}_\Sigma)$ for any choice of polarization $V \in C_\Sigma(A)$. The polarization class $C_\Sigma(A)$ is uniquely determined by the tangential components of the external potential A on Σ. When regarding the Dirac evolution from one Cauchy surface Σ to Σ', another choice of "coordinates" $V' \in C_{\Sigma'}(A)$ has to be made. Then one yields an evolution operator $\tilde{U}^A_{\Sigma'\Sigma} : \mathcal{F}(V,\mathcal{H}_\Sigma) \to \mathcal{F}(V',\mathcal{H}_{\Sigma'})$ which is unique up to an arbitrary phase. Transition probabilities $|\langle\Psi, \tilde{U}^A_{\Sigma'\Sigma}\Phi\rangle|^2$ for $\Psi \in \mathcal{F}(V',\mathcal{H}_{\Sigma'})$ and $\Phi \in \mathcal{F}(V,\mathcal{H}_\Sigma)$ are well-defined and unique without the need of a renormalization method. Finally, for a family of Cauchy surfaces $(\Sigma_t)_{t\in\mathbb{R}}$ that interpolates smoothly between Σ and Σ' one can also infer an infinitesimal version of how the external potential A changes the polarization in terms of the flow parameter t; see Theorem 2.6 in [6].

We remark that the kernel of the orthogonal projector corresponding to a polarization in $\mathrm{C}_\Sigma(A)$, which can be interpreted as a distribution, is frequently called *two-point function*. Two kernels belonging to two polarizations in the same class $\mathrm{C}_\Sigma(A)$ may differ by a square-integrable kernel. This stands in contrast to the so-called Hadamard property (see, e.g., [19]) which allows changes with $\mathcal{C}^\infty$ kernels as freedom in two-point functions.

3 An Explicit Construction of the Evolution Operator

The argument in Sect. 2 that ensures the existence of dynamics on varying Fock spaces is quite abstract. In this section we present a more direct approach that is also closer to Dirac's original picture in describing infinite particle wave functions like in (2). As discussed, the infinitely many particles are also present in the usual Fock space formalism but commonly hidden by use of normal ordering. But since the very obstacle in a straight-forward construction of the evolution operator is due to their presence, it seems to make sense to work with a formalism that makes them apparent. One such formalism, introduced in Section 2 of [4], employs so-called infinite wedge spaces and will be used in the following.

To leave our discussion general, let $\mathcal{H}$ be a one-particle Hilbert space (e.g., $\mathcal{H} = \mathcal{H}_\Sigma$ as in Sect. 2) and let $V \in \mathtt{Pol}(\mathcal{H})$ be a polarization thereof. The Dirac sea corresponding to that choice of polarization can be represented, using any orthonormal basis $(\varphi_n)_{n\in\mathbb{N}}$ that spans V, by the infinite wedge product

$$\Lambda\Phi = \varphi_1 \wedge \varphi_2 \wedge \varphi_3 \wedge \ldots, \tag{26}$$

i.e., the anti-symmetric product of all wave functions φ_n, $n \in \mathbb{N}$. Slightly more general, it suffices if $(\varphi_n)_{n\in\mathbb{N}}$ is only *asymptotically* orthonormal in the sense that the infinite matrix $(\langle\varphi_n, \varphi_m\rangle)_{n,m\in\mathbb{N}}$ has a (Fredholm) determinant, i.e., that it differs from the identity only by a matrix that has a trace. The reason for this property will become clear when introducing the scalar product of two infinite wedge products.

In order to keep the formalism short, we encode the basis $(\varphi_n)_{n\in\mathbb{N}}$ by a bounded linear operator

$$\Phi : \ell \to \mathcal{H}, \qquad \Phi\, e_n = \varphi_n \tag{27}$$

on a Hilbert space ℓ. The role of ℓ is only that of an index space, and one example we have in mind is $\ell = \ell^2(\mathbb{N})$, i.e., the space of square summable sequences where the vectors e_n, $n \in \mathbb{N}$, denote the canonical basis. In this language, the asymptotic orthonormality requirement from above can be rewritten as $\Phi^*\Phi \in \mathrm{id}_\ell + I_1(\ell)$, where $I_1(\ell)$ is the space of bounded linear maps $\ell \to \ell$ which have a trace, the so-called *trace class*. We will also write $\Lambda\Phi = \varphi_1 \wedge \varphi_2 \wedge \ldots$ which denotes the infinite wedge product (26) and refer to all such Φ as *Dirac seas*.

Given another Dirac sea Ψ with $\psi_n = \Psi e_n$, $n \in \mathbb{N}$, the pairing that will later become a scalar product

$$\langle\Lambda\Psi, \Lambda\Phi\rangle = \langle\psi_1 \wedge \psi_2 \wedge \ldots, \varphi_1 \wedge \varphi_2 \wedge \ldots\rangle = \det(\langle\psi_n, \varphi_m\rangle)_{nm} = \det \Psi^*\Phi \tag{28}$$

is well-defined if $\Psi^*\Phi$ has a determinant, which is the case if $\Psi^*\Phi \in \mathrm{id}_\ell + I_1(\ell)$. Thus, it makes sense to build a Fock space, referred to as "infinite wedge space $\mathcal{F}_{\Lambda\Phi}$", based on a basis encoded by Φ. It is defined by the completion w.r.t. the

pairing (28) of the space of *formal* linear combinations of all such Ψ; see Section 2.1 in [4] for a rigorous construction. This space consists of the sea wave function $\Lambda\Phi$, its excitations $\Lambda\Psi$ that form a generating set, and superpositions thereof. An example excitation analogous to (5) representing an electron-positron pair with electron wave function $\chi \in V^\perp$ and positron wave function $\varphi_1 \in V$ is given by

$$\Lambda\Psi = \chi \wedge \varphi_2 \wedge \varphi_3 \wedge \varphi_4 \wedge \dots . \tag{29}$$

Note, however, that mathematically Φ is not distinguished as "the one vacuum" state as it turns out that $\mathcal{F}_{\Lambda\Phi} = \mathcal{F}_{\Lambda\Psi}$ if and only if $\Psi^*\Phi$ has a determinant, i.e., if the scalar product $\langle \Lambda\Psi, \Lambda\Phi\rangle$ in (28) is well-defined. This is due to the fact that $\Psi \sim \Phi :\Leftrightarrow \Psi^*\Phi \in \mathrm{id}_\ell + I_1(\ell)$ is an equivalence relation on the set of all Dirac seas; see Corollary 2.9 in [4].

Next, let us consider another one-particle Hilbert space $\mathcal{H}'$ und a one-particle unitary operator $U : \mathcal{H} \to \mathcal{H}'$ such as the one-particle Dirac evolution operator $U^A_{\Sigma'\Sigma}$. To infer from this a corresponding evolution of the Dirac seas, we define a canonical operation from the left as follows

$$\mathcal{L}_U : \mathcal{F}_{\Lambda\Phi} \to \mathcal{F}_{\Lambda U\Phi}, \qquad \mathcal{L}_U \Lambda\Psi := \Lambda U\Psi = (U\psi_1) \wedge (U\psi_2) \wedge \dots . \tag{30}$$

Here, Ψ is taken from the generating set of Dirac seas fulfilling $\Psi^*\Phi \in 1 + I_1(\ell)$; see Section 2.2 in [4]. That the range of $\mathcal{L}_U$ is $\mathcal{F}_{\Lambda U\Phi}$ is due to the fact that $\Psi^*\Phi$ has a determinant if and only if $(U\Psi)^*(U\Phi)$ does. Such a map $\mathcal{L}_U$ represents an evolution operator from one infinite wedge space into another that in the sense of (6) also complies with the previously discussed lift condition (7).

Nevertheless, the construction of the evolution operator for the Dirac seas does not end here because the target space $\mathcal{F}_{\Lambda U\Phi}$ in (30) is completely implicit, and hence, $\mathcal{L}_U$ alone is not very helpful. On the contrary, relying on the observations made in Sect. 2, physics should allow us to decide beforehand between which infinite wedge spaces the evolution operator should be implemented. Consider the example situation of

$$\begin{gathered} \text{an evolution operator } U = U^A_{\Sigma'\Sigma} \text{ from Theorem 2.3,} \\ \mathcal{H} = \mathcal{H}_\Sigma, \quad V \in \mathtt{Pol}(\mathcal{H}_\Sigma), \quad \Phi : \ell \to \mathcal{H}_\Sigma \text{ such that range } \Phi = V, \\ \mathcal{H}' = \mathcal{H}_{\Sigma'}, \quad V' \in \mathtt{Pol}(\mathcal{H}_{\Sigma'}), \quad \Phi' : \ell' \to \mathcal{H}_{\Sigma'} \text{ such that range } \Phi' = V'. \end{gathered} \tag{31}$$

In this situation one would wish for an evolution operator of the form $\tilde{U} : \mathcal{F}_{\Lambda\phi} \to \mathcal{F}_{\Lambda\Phi'}$ instead of $\tilde{U} : \mathcal{F}_{\Lambda\phi} \to \mathcal{F}_{\Lambda U\Phi}$. If we are not in the lucky case $\mathcal{F}_{\Lambda\Phi'} = \mathcal{F}_{\Lambda U\Phi}$, there are two ways in which the equality may fail. First, Corollary 2.5 suggests that polarization V and V' must be elements of the appropriate polarization classes, more precisely, $V \in C_\Sigma(A)$ and $V' \in C_{\Sigma'}(A)$. However, there is a more subtle obstacle as for $\mathcal{F}_{\Phi'} = \mathcal{F}_{\Lambda U\Phi}$ to hold we need to ensure that $\langle \Phi', U\Phi\rangle$ is well-defined, which

even for $\ell = \ell'$ and admissible V and V' does need not to be the case. Thus, in general $U\Phi$ and Φ' belong to entirely different infinite wedge spaces as the choice of orthonormal bases encoded in Φ and Φ' was somehow arbitrary. However, let $\Psi : \ell \to \mathcal{H}'$ be another Dirac sea with range $\Psi = V'$, then there is a unitary $R : \ell' \to \ell$ such that $\Phi' = \Psi R$. The action of R gives rise to a unitary operation from the right $\mathcal{R}_R$ characterized by

$$\mathcal{R}_R : \mathcal{F}_{\Lambda\Psi} \to \mathcal{F}_{\Lambda\Psi R}, \qquad \mathcal{R}_R \, \Lambda\tilde{\Psi} = \Lambda(\tilde{\Psi} R) \tag{32}$$

for all $\tilde{\Psi} : \ell \to \mathcal{H}'$ in the generating system of $\mathcal{F}_{\Lambda\Psi}$, which connects the infinite wedge spaces $\mathcal{F}_{\Lambda\Psi}$ and $\mathcal{F}_{\Lambda\Phi'}$. The spaces $\mathcal{F}_{\Lambda\Psi}$ and $\mathcal{F}_{\Lambda\Phi'}$ coincide if and only if $\ell = \ell'$ and R has a determinant. Slightly more generally, it suffices if R is only *asymptotically* unitary in the sense that R^*R has a non-zero determinant. Then the operation from the right $\det(R^*R)^{-1/2}\mathcal{R}_R$ is unitary. Whether there is a unitary $R : \ell' \to \ell$ in the situation of example (31) above such that $\mathcal{F}_{\Lambda U\Phi R} = \mathcal{F}_{\Lambda\Phi'}$ is answered by the next theorem. It can be seen as yet another version of the Shale and Stinespring's Theorem:

Theorem 3.11 (Theorem 2.26 of [4]) *Let $\mathcal{H}, \ell, \mathcal{H}', \ell'$ be Hilbert spaces, $V \in \mathtt{Pol}(\mathcal{H})$ and $V' \in \mathtt{Pol}(\mathcal{H}')$ polarizations, $\Phi : \ell \to \mathcal{H}$ and $\Phi' : \ell' \to \mathcal{H}'$ Dirac seas such that* range $\Phi = V$ *and* range $\Phi' = V'$. *Then the following statements are equivalent:*

(a) The off-diagonals $P^{V'^{\perp}} U P^{V}$ and $P^{V'} U P^{V^{\perp}}$ are Hilbert-Schmidt operators.
(b) There is a unitary $R : \ell' \to \ell$ such that $\mathcal{F}_{\Lambda\Phi'} = \mathcal{F}_{\Lambda U\Phi R}$.

Coming back to the example (31) from above, in the case $V \in C_\Sigma(A)$ and $V' \in C_{\Sigma'}(A)$, i.e., that the chosen polarization belong to the admissible classes of polarizations, condition (a) of Theorem 3.11 is fulfilled, which implies the existence of a unitary map $R : V' \to V$ such that the evolution operator

$$\tilde{U}^A_{V,\Sigma;V'\Sigma'} : \mathcal{F}_{\Lambda\Phi} \to \mathcal{F}_{\Lambda\Phi'}, \qquad \tilde{U}^A_{V,\Sigma;V'\Sigma'} = \mathcal{R}_R \circ \mathcal{L}_{U^A_{\Sigma'\Sigma}} \tag{33}$$

is well-defined and unitary. An immediate question is of course how many such maps exist, and it turns out that any other operation from the right $\mathcal{R}_{R'}$ for which $\mathcal{R}_{R'} \circ \mathcal{L}_U : \mathcal{F}_{\Lambda\Phi} \to \mathcal{F}_{\Lambda\Phi'}$ is well-defined and unitary fulfills $\tilde{U}^A_{V,\Sigma;V'\Sigma'} = e^{i\theta}\, \mathcal{R}_{R'} \circ \mathcal{L}_U$ for some $\theta \in \mathbb{R}$; see [4, Corollary 2.28]. Now Φ and Φ' are Dirac seas in which all states in V and V' are occupied, respectively. A canonical choice for their representation is to choose $\ell = V$, $\ell' = V'$, and to define the inclusion maps $\Phi : V \hookrightarrow \mathcal{H}_\Sigma$, $\Phi v = v$ for all $v \in V$, and $\Phi' : V' \hookrightarrow \mathcal{H}_{\Sigma'}$, $\Phi' v' = v'$ for all $v' \in V'$. In this case there is a canonical isomorphism between the spaces $\mathcal{F}_{\Lambda\Phi}$ and $\mathcal{F}_{V,\Sigma}$ as well as between $\mathcal{F}_{\Lambda\Phi'}$ and $\mathcal{F}_{V',\Sigma'}$. Hence, we are again in the situation of Corollary 2.5. We can identify the evolution of the Dirac seas only up to a phase $\theta \in \mathbb{R}$. However, now we have a more direct construction at hand which identifies the involved degrees of freedom:

(a) The choice of particular polarizations $V \in C_\Sigma(A)$ and $V' \in C_{\Sigma'}(A)$.
(b) The choice of particular bases encoded in Φ and Φ'.

The restriction of the polarizations to polarization classes in (a) has been discussed in Sect. 2. Moreover, choice (b) can be given a quite intuitive picture coming from Dirac's original idea that the motion deep down in the sea should be irrelevant when studying the excitations on its "surface". Clearly, when a sea wave function $\Lambda\Psi \in \mathcal{F}_{\Lambda\Phi}$, which could represent an excitation w.r.t. $\Lambda\Phi$, is evolved from Σ to $\Lambda\Psi'$ on Σ', clearly also the particles deep down in the sea will "move". Since there are infinitely many it will be impossible to directly compare Ψ' with Ψ in general. Writing $U = U^A_{\Sigma'\Sigma}$ in matrix notation

$$U = \begin{pmatrix} U_{++} & U_{+-} \\ U_{-+} & U_{--} \end{pmatrix} = \begin{pmatrix} P^{V'^\perp}_{\Sigma'} U P^{V^\perp}_{\Sigma} & P^{V'^\perp}_{\Sigma'} U P^{V}_{\Sigma} \\ P^{V'}_{\Sigma'} U P^{V^\perp}_{\Sigma} & P^{V'}_{\Sigma'} U P^{V}_{\Sigma} \end{pmatrix}, \tag{34}$$

the motion deep down in the sea is governed by U_{--}. Now, if according to Dirac's original idea the motion deep down in the sea can be considered irrelevant for the behavior of the excitations on its surface one should still be able to compare $\Lambda\Psi'$ to $\Lambda\Psi$ when reversing the motion deep down in the sea with $(U_{--})^{-1}$. If U is for example sufficiently close to the identity this can be done explicitly since then U_{--} has an inverse $R = (U_{--})^{-1}$. As we shall see now, the inversion of the motion deep down in the sea can be implemented by means of an operation from the right $\mathcal{R}_R$. For R to induce an operation from the right it has to be asymptotically orthonormal, i.e., R^*R must have a determinant. Recall that condition (a) in Theorem 3.11 states that the off-diagonals U_{+-} and U_{-+} are Hilbert-Schmidt operators. Thanks to $U^*U = \mathrm{id}_{\mathcal{H}}$ the identity

$$U^*_{--}U_{--} = \mathrm{id}_V - (U^*)_{-+}U_{+-} \tag{35}$$

holds, and since the product of two Hilbert-Schmidt operators has a trace, one finds $U^*_{--}U_{--} \in \mathrm{id}_V + I_1(V)$. Thus, $U^*_{--}U_{--}$ and then also R^*R have determinants. Note that in general $\det(R^*R) \neq 1$, which implies that $\mathcal{R}_R$ may fail to be unitary up to the factor $\det|R|$. By definition one finds

$$\mathcal{R}_R \circ \mathcal{L}_U \mathcal{F}_{\Lambda\Phi} = \mathcal{F}_{\Lambda U\Phi R} = \mathcal{F}_{\Lambda\Phi'} \tag{36}$$

because $\Phi'^* U \Phi R = P^{V'}(U_{+-} + U_{--})R = \mathrm{id}_{V'}$, and therefore, has a determinant. In consequence, we obtain the unitary Dirac evolution

$$\begin{aligned} \tilde{U}^A_{V,\Sigma;V'\Sigma'} &: \mathcal{F}_{\Lambda\Phi} \to \mathcal{F}_{\Lambda\Phi'}, \\ \tilde{U}^A_{V,\Sigma;V'\Sigma'} &= \det|(U^A_{\Sigma'\Sigma})_{--}|\, \mathcal{R}_{[(U^A_{\Sigma'\Sigma})_{--}]^{-1}} \circ \mathcal{L}_{U^A_{\Sigma'\Sigma}}, \end{aligned} \tag{37}$$

which implements both the forward evolution of the whole Dirac sea and the backward evolution of the states deep down in the sea.

4 The Charge Current and the Phase of the Evolution Operator

Although the construction of the second-quantized evolution operator according to the above program is successful, it fails to identify the phase. This short-coming has no effect on the uniqueness of transition probabilities but it turns out that the charge current depends directly on this phase. One way to see that is from Bogolyubov's formula of the current

$$J^\mu(x) = i\,\tilde{U}^A_{V_{\text{in}},\Sigma_{\text{in}};V_{\text{out}}\Sigma_{\text{out}}}\,\frac{\delta}{\delta A_\mu(x)}\,\tilde{U}^A_{V_{\text{out}},\Sigma_{\text{out}};V_{\text{in}},\Sigma_{\text{in}}}, \tag{38}$$

where Σ_{out} is a Cauchy surface in the remote future of the support of A such that $\Sigma_{\text{out}} \cap \text{supp}A = \emptyset$. Changing the evolution operator by an A-dependent phase generates another summand on the right hand side of (38) by the chain rule. Until some phase is distinguished, (38) has no particular physical meaning as charge current. Nevertheless, all possible currents can be derived from (38) given an evolution operator and a particular phase. Therefore, the situation is better than in standard QED. There, the charge current is a quantity whose formal perturbation series leads to several divergent integrals which have to be taken out by hand until only a logarithmic divergence is left, which in turn is remedied by means of charge renormalization. On the contrary, here, the currents are well-defined and in a sense the correct one only needs to be identified by determining the phase of the evolution operator. As already envisioned in [28] and discussed by [15, 22], this may be done by imposing extra conditions on the evolution operator. One of them is clearly the following property. For any choice of a future oriented foliation of space-time into a family of Cauchy surfaces $(\Sigma_t)_{t\in\mathbb{R}}$ and polarizations $V_t \in C_{\Sigma_t}(A)$, $t \in \mathbb{R}$, the assigned phase of the evolution operator $\tilde{U}^A(t_1,t_0) = \tilde{U}^A_{\Sigma_{t_1},V_{t_1};\Sigma_{t_0},V_{t_0}}$ constructed in Sect. 3 should be required to fulfill $\tilde{U}(t_1,t_0) = \tilde{U}(t_1,t)\tilde{U}(t,t_0)$. Other constraints come from the fact that $J^\mu(x)$ must be Lorentz and gauge covariant, and its vacuum expectation value for $A = 0$ should be zero. The hope is that the collection of all such physical constraints restrict the possible currents (38) to a class which can be parametrized by a real number only, the electric charge of the electron. In the case of equal-time hyperplanes one possible choice of the phase was given by Mickelsson via a parallel transport argument [23]. On top of the nice geometric construction and despite the fact that there are still degrees of freedom left, Mickelsson's current agrees with conventional perturbation theory up to second order. The aim of this program is to settle the question which conditions are required to identify the charge current upon changes of the value of the electric charge.

Acknowledgements This work has partially been funded by the Elite Network of Bavaria through the JRG "Interaction between Light and Matter".

References

1. C.D. Anderson, The positive electron. Phys. Rev. **43**(6), 491–494 (1933)
2. C. Bär, N. Ginoux, F. Pfäffle, *Wave Equations on Lorentzian Manifolds and Quantization* (European Mathematical Society, Zürich, 2007)
3. D.-A. Deckert, *Electrodynamic Absorber Theory – A Mathematical Study* (Der Andere Verlag, 2010)
4. D.-A. Deckert, D. Dürr, F. Merkl, M. Schottenloher, Time-evolution of the external field problem in quantum electrodynamics. J. Math. Phys. **51**(12), 122301 (2010)
5. D.-A. Deckert, F. Merkl, Dirac equation with external potential and initial data on Cauchy surfaces. J. Math. Phys. **55**(12), 122305 (2014)
6. D.-A. Deckert, F. Merkl, *External Field QED on Cauchy Surfaces* (In preparation)
7. J. Derezinski, C. Gérard, *Mathematics of Quantization and Quantum Fields* (Cambridge University Press, Cambridge, 2013)
8. J. Dimock, Dirac quantum fields on a manifold. Trans. Am. Math. Soc. **269**(1), 133–147 (1982)
9. P.A.M. Dirac, Theorie du Positron, *Selected Papers on Quantum Electrodynamics*, ed. by J. Schwinger (Dover Publications Inc., New York, 1934)
10. H. Fierz, G. Scharf, Particle interpretation for external field problems in QED. Helv. Phys. Acta. Phys. Theor. **52**(4), 437–453 (1980)
11. F. Finster, *The Continuum Limit of Causal Fermion Systems* (In preparation). Book based on the preprints arXiv:0908.1542; arXiv:1211.3351; arXiv:1409.2568
12. F. Finster, J. Kleiner, *Causal Fermion Systems as a Candidate for a Unified Physical Theory.* arXiv:1502.03587
13. F. Finster, J. Kleiner, J.-H. Treude, *An Introduction to the Fermionic Projector and Causal Fermion Systems* (In preparation)
14. F. Finster, J. Kleiner, J.-H. Treude, An introduction to the fermionic projector and causal fermion systems. Trans. Am. Math. Soc. (2012)
15. J.M. Gracia-Bondia, The phase of the scattering matrix. Phys. Lett. B **482**(1–3), 315–322 (2000)
16. P. Gravejat, C. Hainzl, M. Lewin, E. Séré, Construction of the Pauli–Villars-Regulated Dirac vacuum in electromagnetic fields. Archiv. Ration. Mech. Anal. **208**(2), 603–665 (2013)
17. W. Greiner, D.A. Bromley, *Relativistic Quantum Mechanics. Wave Equations*, 3rd edn. (Springer, Berlin/New York, 2000)
18. F. John, *Partial Differential Equations* (Springer, New York, 1982)
19. B.S. Kay, R.M. Wald, Theorems on the uniqueness and thermal properties of stationary, nonsingular, quasifree states on spacetimes with a bifurcate killing horizon. Phys. Rep. **207**(2), 49–136 (1991)
20. O. Klein, Die Reflexion von Elektronen an einem Potentialsprung nach der relativistischen Dynamik von Dirac. Z. für Phys. **53**(3–4), 157–165 (1929)
21. E. Langmann, J. Mickelsson, Scattering matrix in external field problems. J. Math. Phys. **37**(8), 3933–3953 (1996)
22. J. Mickelsson, Vacuum polarization and the geometric phase: gauge invariance. J. Math. Phys. **39**(2), 831—837 (1998)
23. J. Mickelsson, The phase of the scattering operator from the geometry of certain infinite-dimensional groups. Lett. Math. Phys. **104**(10), 1189–1199 (2014)
24. P. Pickl, D. Dürr, Adiabatic pair creation in heavy-ion and laser fields. Europhys. Lett. **81**(4), 40001 (2008)
25. H. Ringström, *The Cauchy Problem in General Relativity* (European Mathematical Society, Zürich, 2009)
26. S.N.M. Ruijsenaars, Charged particles in external fields. I. Classical theory. J. Math. Phys. **18**(4), 720–737 (1977)
27. S.N.M. Ruijsenaars, Charged particles in external fields. II. The quantized Dirac and Klein-Gordon theories. Commun. Math. Phys. **52**(3), 267–294 (1977)

28. G. Scharf, *Finite Quantum Electrodynamics: The Causal Approach*, 2nd edn. (Springer, Berlin/New York, 1995)
29. E. Schrödinger, Über die kräftefreie Bewegung in der relativistischen Quantenmechanik. Berliner Ber. 418–428 (1930)
30. D. Shale, W.F. Stinespring, Spinor representations of infinite orthogonal groups. J. Math. Mech. **14**, 315–322 (1965)
31. M.E. Taylor, *Partial Differential Equations III* (Springer, New York, 2011)

Super Riemann Surfaces and the Super Conformal Action Functional

Enno Keßler

Contents

Abstract Riemann surfaces are two-dimensional manifolds with a conformal class of metrics. It is well known that the harmonic action functional and harmonic maps are tools to study the moduli space of Riemann surfaces. Super Riemann surfaces are an analogue of Riemann surfaces in the world of super geometry. After a short introduction to super differential geometry we will compare Riemann surfaces and super Riemann surfaces. We will see that super Riemann surfaces can be viewed as Riemann surfaces with an additional field, the gravitino. An extension of the harmonic action functional to super Riemann surfaces is presented and applications to the moduli space of super Riemann surfaces are considered.

Keywords Super symmetry • Super geometry • Super Riemann surfaces • Non-linear super symmetric sigma model

Mathematics Subject Classification (2010). 31C11, 30F15, 32G15, 58A50, 81T30, 83E30, 83E50

E. Keßler (✉)
Max-Planck-Institut für Mathematik in den Naturwissenschaften, Inselstraße 22, 04103 Leipzig, Germany
e-mail: kessler@mis.mpg.de

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_17

The theory of Riemann surfaces is a very old and very interesting topic. Since the end of the nineteenth century Riemann surfaces have been explored with different approaches from different areas of mathematics ranging from algebraic geometry to analysis. In particular the description of Riemann surfaces in terms of conformal classes of metrics and the Teichmüller theory has an interesting connection to harmonic maps and the harmonic action functional (see, for example, [14]). Harmonic maps from Riemann surfaces are particular non-linear sigma models.

In contrary, Super Riemann surfaces are a rather new topic. They appeared in the context of super gravity and super string theory around 1985, see [10, 22]. Super Riemann surfaces have been formalized using the language of super geometry (see e.g. [20]), an extension of differential or algebraic geometry. Super Riemann surfaces are particular complex super manifolds of complex dimension $1|1$. Even though they possess one even and one odd dimension they are said to behave in certain regards as if they were one-dimensional. Different approaches from the theory of Riemann surfaces have been "superized", such as uniformization [4] and universal deformation spaces [19].

The approach to super Riemann surfaces via super conformality and a super harmonic action functional is very interesting for physics, as it appears in a super symmetric non-linear sigma model. In [2, 7] it was proposed to consider a super symmetric extension of the harmonic action functional $A(\varphi, g)$ where both the metric g and the field φ get a super partner, ψ and χ respectively. This particular super symmetric non-linear sigma model is relevant for string theory and super gravity.

It was conjectured that a super Riemann surface M can be described by a metric g and the super partner of the metric, called gravitino χ on a two dimensional manifold $|M|$. The action of the non-linear super symmetric sigma model would then be an integral over the super manifold M, resembling the harmonic action functional on $|M|$. Mathematically this leads to a different approach to the moduli space of super Riemann surfaces. In a talk at the conference "Quantum Mathematical Physics" in fall 2014 I presented my research to make precise the relation between the super symmetric non-linear sigma model and super Riemann surfaces. The present paper is a written up version of that talk.

The first chapter gives a brief introduction to the necessary parts of super geometry. We focus mainly on the local theory, that is the building block $\mathbb{R}^{m|n}$. Motivation is given by a toy example.

In the second section we will see how super Riemann surfaces can be reduced to Riemann surfaces with an additional gravitino field. A possible super Teichmüller theory is discussed.

In the third section, the extension of the classical harmonic action functional to super Riemann surfaces is given. Using the results of the second section it is possible to formulate the super harmonic action functional as an integral over a two-dimensional manifold. Symmetries of the action functional can be explained with the help of the geometry of super Riemann surfaces. In analogy to the case of

Riemann surfaces, it is expected that the super harmonic action functional may help to understand super Teichmüller space.

1 Super Geometry

The theory of super manifolds was developed in the 1970s and 1980s in order to provide a geometrical framework for super symmetric theories in high-energy physics. Already at that time two different approaches were developed. One approach is to extend the definition of manifolds in terms of charts by replacing the real numbers by certain Grassmann algebras, see e.g. [23]. The other approach is inspired by algebraic geometry. It puts emphasis on functions rather than on points. An early overview article for this approach is [20]. It is proven in [1] that both approaches coincide. We will use here the algebraic approach to super manifolds and certain generalizations given below.

Example 1.1 We will motivate and illustrate most definitions in this section by help of the following toy model, inspired by [5, §1.3]. Let φ and ψ (classical) fields on $\mathbb{R}$. The main motivation for super geometry is to unify φ and ψ into one object

$$\Phi = \varphi + \eta\psi \tag{1}$$

and to be able to interpret super symmetry, i.e. transformations of the following type

$$\delta\varphi = q\psi \qquad\qquad \delta\psi = q\partial_x\varphi \tag{2}$$

in a geometric way. To this end one needs to extend the geometrical setting from the domain $\mathbb{R}$ to $\mathbb{R}^{1|1}$, where the objects Φ, η and the super symmetry transformations get a precise meaning.

Recall that a locally ringed space M is a pair $(\|M\|, \mathcal{O}_M)$, where $\|M\|$ is a topological space and $\mathcal{O}_M$ a sheaf of rings on M, see [12, §0.4]. Sections of $\mathcal{O}_M$ are called functions. A homomorphism of ringed spaces $\varphi\colon M \to N$ is a pair $\varphi = (\|\varphi\|, \varphi^{\#})$ consisting of a homomorphism $\|\varphi\|\colon \|M\| \to \|N\|$ of the underlying topological spaces and a sheaf homomorphism $\varphi^{\#}\colon \mathcal{O}_N \to \mathcal{O}_M$ over φ.

Definition 1.2 We denote by $\mathbb{R}^{m|n}$ the ringed space given by the topological space $\mathbb{R}^m$ together with the sheaf of functions

$$\mathcal{O}_{\mathbb{R}^{m|n}} = C^\infty(\mathbb{R}^m, \mathbb{R}) \otimes \Lambda_n$$

where Λ_n is a real Grassmann algebra in n generators. A super manifold M is a ringed space which is locally isomorphic to $\mathbb{R}^{m|n}$. We say that M has m even and n odd dimensions, or that M is of dimension $m|n$. A homomorphism of super manifolds $\varphi\colon M \to N$ is a homomorphism of locally ringed spaces.

Let $x^1, \ldots, x^m$ be the standard coordinate functions on $\mathbb{R}^m$ and $\eta^1, \ldots, \eta^n$ generators of the Grassmann algebra Λ_n. We call the tuple $(X^A) = (x^a, \eta^\alpha)$ of functions on $\mathbb{R}^{m|n}$ coordinates of $\mathbb{R}^{m|n}$. Any function $f \in \mathcal{O}_{\mathbb{R}^{m|n}}$ can be expressed as a finite expansion in the odd coordinates η^α:

$$f = \sum_{\underline{\gamma}} \eta^{\underline{\gamma}} f_{\underline{\gamma}}(x) = f_0 + \eta^\alpha f_\alpha + \ldots$$

Here the summation runs over all odd multiindices $\underline{\gamma}$. The functions $f_{\underline{\gamma}}$ are ordinary functions on $\mathbb{R}^m$.

Notice that $\mathcal{O}_{\mathbb{R}^{m|n}}$ inherits a $\mathbb{Z}_2$ grading from the Grassmann algebra Λ_n. We will call elements of $\mathcal{O}_{\mathbb{R}^{m|n}}$ of parity 0 even and elements of parity 1 odd. We use here and in the following the convention, that small roman letters are used for even objects, small greek letters for odd objects and capital letters for even and odd objects together.

In contrast to the theory of manifolds, not every function $f \in \mathcal{O}_{\mathbb{R}^{m|n}}$ can be seen as a map $\mathbb{R}^{m|n} \to \mathbb{R}$. This is a consequence of the graduation of the structure sheaf $\mathcal{O}_{\mathbb{R}^{n|m}}$. By [20, Theorem 2.17], maps between super domains $U \subseteq \mathbb{R}^{m|n}$ and $V \subseteq \mathbb{R}^{p|q}$ can be given in terms of coordinates.

Example 1.3 A first possible interpretation for Eq. (1) would be that

$$\Phi = \varphi + \eta\psi$$

is a function on $\mathbb{R}^{1|1}$ with coordinates (x, η). This would however restrict φ and ψ to be smooth functions on $\mathbb{R}$. Even though it looks like a drawback at first sight, the correct way is to consider maps $\Phi\colon \mathbb{R}^{1|1} \to \mathbb{R}$. Let r be a coordinate function on $\mathbb{R}$. The map Φ is then completely determined by the pullback $\Phi^\# r$ which is an even function on $\mathbb{R}^{1|1}$ because the ring homomorphisms $\Phi^\#$ preserve automatically the $\mathbb{Z}_2$-parity of the functions:

$$\Phi^\# r = \varphi(x) + \eta\psi(x)$$

However, if $\Phi^\# r$ is even the function $\psi(x)$ has to be zero. For the applications we have in mind $\psi(x)$ is certainly expected to be non-zero. Therefore we need to consider a family of maps Φ parametrized by a super manifold B, i.e. a map that makes the following diagram commutative:

$$\begin{array}{ccc} \mathbb{R}^{1|1} \times B & \xrightarrow{\Phi} & \mathbb{R} \times B \\ & {\scriptstyle p_B} \searrow \quad \swarrow {\scriptstyle p_B} & \\ & B & \end{array}$$

Such a map is again completely determined by the pullback $\Phi^{\#}r$ which is this time an even function on $\mathbb{R}^{1|1} \times B$:

$$\Phi^{\#}r = \varphi(x) + \eta\psi(x)$$

Here the coefficients functions $\varphi(x)$ and $\psi(x)$ are functions on $\mathbb{R}^{1|0} \times B$. We suppress the B-dependence in the notation. As $\Phi^{\#}r$ is even, and η is odd, also $\psi(x)$ has to be odd. This is possible if the base B possesses odd dimensions.

The Example 1.3 motivates the following definition:

Definition 1.4 ([20]) A submersion $p_M: M \to B$ of super manifolds is also called a family of super manifolds over B. A morphism f of families of super manifolds from $p_M: M \to B$ to $p_N: N \to B$ is a morphism $f: M \to N$ such that $p_N \circ f = p_M$. Any super manifold is a family over $\mathbb{R}^{0|0} = (\{pt\}, \mathbb{R})$. Any family is locally a projection $\mathbb{R}^{m|n} \times B \to B$. We call $m|n$ the dimension of the family.

According to [6, Remark 2.6.(v)] it is not necessary to fix B. However B is always supposed to be "big enough", see Example 1.3. Henceforth, all super manifolds and maps of super manifolds are implicitly to be understood as families of super manifolds and morphisms of families of super manifolds. In particular, also $\mathbb{R}^{m|n}$ is to be understood as the trivial family $\mathbb{R}^{m|n} \times B$.

Remark 1.5 Another quite popular approach to super manifolds is to use the functor of points. Full discussions of this approach can be found in [24]. An advantage of this approach is that one can treat infinite dimensional super manifolds. Infinite dimensional manifolds can not be treated in the ringed-space approach. However non-trivial families of super manifolds are usually not in the scope of the functor of points approach. We will see in the next chapter, that we need non-trivial families of super manifolds for the study of moduli spaces.

It is possible to extend a large part of differential geometry to super manifolds, see e.g. [3, 6, 20]. In particular there are appropriate definitions of vector bundles, tangent bundles, Lie groups and principle bundles.

Example 1.6 Let (x^a, η^α) be coordinates for $\mathbb{R}^{m|n}$. Any vector field V on $\mathbb{R}^{m|n}$ are $\mathcal{O}_{\mathbb{R}^{m|n}}$-linear combination of the partial derivatives in coordinate directions:

$$V = V^a \partial_{x^a} + V^\alpha \partial_{\eta^\alpha}$$

A particular vector field on $\mathbb{R}^{1|1}$ is given by the even vector field $Q = q\left(\partial_\eta - \eta\partial_x\right)$. It acts on the function $\Phi^{\#}r$ by

$$Q\Phi^{\#}r = q\left(\partial_\eta - \eta\partial_x\right)(\varphi(x) + \eta\psi(x)) = q\psi(x) + \eta q\partial_x\varphi$$

The coefficients of $Q\Phi^{\#}r$ reproduce the super symmetry transformations from Eq. (2). Consequently, the infinitesimal super diffeomorphism given by the vector field Q can be identified with the super symmetry transformations (2).

In order to study the relation between super manifolds and ordinary manifolds, we need the concept of an underlying even manifold.

Definition 1.7 ([16]) Let $M = (\|M\|, \mathcal{O}_M)$ be a family of super manifolds of dimension $m|n$ over B. A family of super manifolds $|M| = (\|M\|, \mathcal{O}_{|M|})$ of dimension $m|0$ together with an embedding of families of super manifolds $i\colon |M| \to M$ that is the identity on the underlying topological space is called an underlying even manifold.

In [16] we have shown that such underlying even manifolds always exist. They are unique, however, only if the odd dimension of B is zero.

Example 1.8 Remember that we have defined the fields $\varphi(x)$ and $\psi(x)$ as coefficients in the coordinate expansion of

$$\Phi^{\#} r = \varphi(x) + \eta\psi(x)$$

with respect to fixed coordinates (x, η), see Example 1.3. This definition is clearly coordinate dependent. A general coordinate change on $\mathbb{R}^{1|1}$ (over B) is given by

$$x = g_0(\tilde{x}) + \tilde{\eta} g_1(\tilde{x}) \qquad \eta = \gamma_0(\tilde{x}) + \tilde{\eta}\gamma_1(\tilde{x})$$

In the coordinates $(\tilde{x}, \tilde{\eta})$ the map Φ is given by

$$\Phi^{\#} r = \varphi(g_0(\tilde{x})) + \gamma_0(\tilde{x})\psi(g_0(\tilde{x})) + \tilde{\eta}\left(\frac{d\varphi}{dx}(g_0(\tilde{x}))g_1(\tilde{x}) + \gamma_1(\tilde{x})\psi(g_0(\tilde{x}))\right)$$

With the help of a chosen embedding $i\colon \mathbb{R}^{1|0} \times B \to \mathbb{R}^{1|1} \times B$ we are able to give a coordinate independent definition of φ and ψ. Let y be the standard coordinate on $\mathbb{R}^{1|0}$ and (x, η) the standard coordinates on $\mathbb{R}^{1|1}$. Any embedding i can be expressed in those coordinates as:

$$i^{\#} x = y \qquad i^{\#}\eta = \xi$$

for some odd function ξ in $\mathcal{O}_{\mathbb{R}^{1|0}\times B}$. At this point it is obvious why the embedding is unique if $B = \mathbb{R}^{0|0}$.

The automorphism of $\mathbb{R}^{1|1} \times B$ given by

$$\tilde{x} = x \qquad \tilde{\eta} = \eta - \xi$$

yields $i^{\#}\tilde{\eta} = 0$.

Define the field $\varphi = \Phi \circ i\colon \mathbb{R}^{1|0} \to \mathbb{R}$. One can assume without loss of generality that the embedding i is given by $i^{\#}\eta = 0$. Then the degree zero coefficient of $\Phi^{\#} r$ coincides with φ:

$$\Phi^{\#} r = \varphi(x) + \eta f_1(x)$$

Note that the choice of i fixes only one component field. Any coordinate change

$$x = \tilde{x} + \tilde{\eta} g_1(\tilde{x}) \qquad \eta = \tilde{x} + \tilde{\eta}\gamma_1(\tilde{x})$$

preserves $\varphi(x)$, but not ψ. Any given embedding i splits all super diffeomorphisms of $\mathbb{R}^{1|1}$ (Eq. (1)) into diffeomorphisms of $\mathbb{R}^{1|0}$ (given by g_0), diffeomorphisms of $\mathbb{R}^{1|1}$ that preserve i (given by g_1 and γ_1), and diffeomorphisms of $\mathbb{R}^{1|1}$ that change i (given by γ_0).

We define the second component field ψ with the help of the vector field $D = \partial_\eta + \eta\partial_x$. The vector field D is characterized by the property that it commutes with the super symmetry vector field Q given in Example 1.6. The definition $\psi = i^*D\Phi$ then assures that ψ is the super partner to φ, because the action of the vector field Q on the component fields is given by

$$\delta\varphi = i^*Q\Phi = q\psi \qquad \delta\psi = i^*QD\Phi = q\partial_x\varphi$$

The definition of ψ given here shows that ψ is a section of $\varphi^*T\mathbb{R}$ and is independent of the chosen coordinates. The vector field D encountered here is crucial for the definition of super Riemann surfaces in the next chapter. The particular structure of super Riemann surfaces will then also assure that, contrary to our toy model here, ψ is a spinor.

Integrals over a super manifold M can be reduced to integrals over $|M|$ via an embedding $i\colon |M| \to M$. Integration is defined for sections of $\operatorname{Ber} T^\vee M$, a generalization of the determinant line bundle. Integration is given in local coordinates (x^a, η^α) such that $i^\#\eta^\alpha = 0$ by

$$\int_{\mathbb{R}^{m|n}} g(x,\eta)[dx^1 \dots dx^m\, d\eta^1 \dots d\eta^n] = \int_{\mathbb{R}^{m|0}} g_{top}(x)\, dx^1 \dots dx^m$$

where g_{top} is the coefficient of $\eta^1 \cdot \dots \cdot \eta^n$ in the coordinate expansion of g.

Example 1.9 In our toy model, a super symmetric action for the fields φ and ψ is given by

$$A(\varphi,\psi) = \frac{1}{2}\int_{\mathbb{R}} \varphi'^2 + \psi\psi'\, dx$$

The action $A(\varphi,\psi)$ can be formulated in terms of super symmetry via an integral over $\mathbb{R}^{1|1}$ where the integrand depends on Φ as follows:

$$A(\varphi,\psi) = A(\Phi) = -\frac{1}{2}\int_{\mathbb{R}^{1|1}} \partial_x\Phi D\Phi[dx\, d\eta]$$

Note that the reduction of the integral over $\mathbb{R}^{1|1}$ to an integral over $\mathbb{R}$ is given with respect to i. However the definition of $A(\Phi)$ does not depend on i. Consequently

the integral $A(\Phi)$ has an additional symmetry, the change of embedding i. An infinitesimal change of embedding i is given by the even vector field $Q = q\left(\partial_\eta - \eta\partial_x\right)$. The super symmetry of $A(\varphi, \psi)$ can thus be interpreted geometrically, in terms of a change of embedding of the underlying even manifold.

2 Super Riemann Surfaces

Super Riemann surfaces are 2|2-dimensional super manifolds with additional structure. They appeared in the 1980s in the context of string theory and super gravity. Early references are [10, 11, 19, 22]. We will see in this section how they can be considered as a generalization of classical Riemann surfaces and give an outlook to a possible super Teichmüller theory.

Let us recall, that there are several different ways to define and study Riemann surfaces. From the viewpoint of complex geometry, Riemann surfaces are 1-dimensional complex manifolds.

In differential geometry one can describe Riemann surfaces as two-dimensional (real) manifolds with additional geometric structure, given by a conformal class of metrics or an almost complex structure. Let $|M|$ be a two-dimensional smooth manifold of genus p. Let furthermore g and $\tilde{g}$ be two Riemannian metrics on $|M|$. Recall that the metrics g and $\tilde{g}$ belong to the same conformal class $[g]$ if there is a positive function Λ such that $g = \Lambda\tilde{g}$. In two dimensions, a conformal class of metrics together with an orientation induces an almost complex structure I by

$$g(IX, Y) = dvol_g(X, Y)$$

for all vector fields X and Y. It is also particular to the two-dimensional case that this almost complex structure is always integrable, i.e. leads to a complex manifold.

Let $f\colon |M| \to |M|$ be a diffeomorphism. The metric spaces $(|M|, g)$ and $(|M|, f^*g)$ are isometric. Consequently the resulting Riemann surfaces are isomorphic and isomorphism classes of Riemann surfaces are described by the quotient of conformal classes up to diffeomorphisms:

$$\mathcal{M}_p = \{\text{conformal classes } [g] \text{ on } |M|\} \,/\, \text{Diff}\,|M| \tag{3}$$

Unfortunately the isomorphism classes of Riemann surfaces cannot be endowed with a manifold structure. However, an infinite cover of this space can be equipped with a manifold structure, the Teichmüller space:

$$\mathcal{T}_p = \{\text{conformal classes } [g] \text{ on } |M|\} \,/\, \text{Diff}_0\,|M| \tag{4}$$

Here $\text{Diff}_0\,|M|$ denotes diffeomorphisms of $|M|$ that are homotopic to the identity. It is a theorem due to Oswald Teichmüller, that the Teichmüller space $\mathcal{T}_p$ is isomorphic to $\mathbb{R}^{6p-6}$.

Infinitesimal deformations of a given Riemann surface $(|M|, g)$ are tangent vectors to the appropriate point in Teichmüller space. Since Riemann surfaces are described here in terms of Riemannian metrics, infinitesimal deformations of Riemann surfaces are given by infinitesimal changes δg of the metric g. Any infinitesimal change of the metric δg can be decomposed into infinitesimal conformal rescaling, Lie derivative of g (infinitesimal diffeomorphism) and "true infinitesimal deformations" of the Riemann surface:

$$\delta g = \lambda g + L_X g + D \tag{5}$$

It can be shown that the true infinitesimal deformations D are holomorphic quadratic differentials, i.e. holomorphic sections of $T^\vee|M| \otimes_{\mathbb{C}} T^\vee|M|$.

Super Riemann surfaces can also be described and studied with more algebraic or more differential geometric methods. After a brief look at the algebraic definition of super Riemann surfaces and its consequences we will turn to a more differential geometric treatment of super Riemann surfaces. We will see that the differential geometric picture allows to describe a super Riemann surface M in terms of a metric g, a spinor bundle S, and a gravitino field χ on an underlying even manifold $|M|$. This is a precise version of a conjecture to be found in [8, 15].

We use here the algebraic definition of super Riemann surfaces given in [19, 22].

Definition 2.1 A super Riemann surface is a $1|1$-dimensional complex super manifold M with a $0|1$-dimensional distribution $\mathcal{D} \subset TM$ such that the commutator of vector fields induces an isomorphism

$$\frac{1}{2}[\cdot,\cdot]\colon \mathcal{D} \otimes_{\mathbb{C}} \mathcal{D} \to TM/\mathcal{D}.$$

Example 2.2 Let (z, θ) be the standard coordinates on $\mathbb{C}^{1|1}$ and define $\mathcal{D} \subset T\mathbb{C}^{1|1}$ by $\mathcal{D} = \langle \partial_\theta + \theta\partial_z \rangle$. The isomorphism $\mathcal{D} \otimes \mathcal{D} \simeq TM/\mathcal{D}$ is explicitly given by

$$[\partial_\theta + \theta\partial_z, \partial_\theta + \theta\partial_z] = 2\partial_z$$

This example is generic since any super Riemann surface is locally of this form, see [19, Lemma 1.2].

The following proposition is an easy consequence of this definition:

Proposition 2.3 (see e.g. [24, Proposition 4.2.2]) *There exists a bijection between the set of super Riemann surfaces over $\mathbb{R}^{0|0}$ and the set of pairs $(|M|, S)$, where S is a spinor bundle over the Riemann surface $|M|$, i.e. $S \otimes_{\mathbb{C}} S = T|M|$.*

Proof As indicated in the Example 2.2, the super Riemann surface M can be covered by coordinate charts (z, θ) such that the holomorphic line bundle $\mathcal{D}$ is generated by

$\partial_\theta + \theta\partial_z$. Suppose (z, θ) and $(\tilde{z}, \tilde{\theta})$ are two pairs of such coordinates. In the formula for the holomorphic change of coordinates

$$\tilde{z} = f(z) \qquad \tilde{\theta} = g(z)\theta \tag{6}$$

the holomorphic functions $f(z)$ and $g(z)$ are related by the condition that $\partial_{\tilde{\theta}} + \tilde{\theta}\partial_{\tilde{z}}$ must be proportional to $\partial_\theta + \theta\partial_z$. One can check that

$$\partial_\theta + \theta\partial_z = g(z)\left(\partial_{\tilde{\theta}} + \tilde{\theta}\partial_{\tilde{z}}\right)$$

if and only if $f'(z) = g(z)^2$. As the unique underlying even manifold is given by $\theta = 0$, the coordinates z induce a complex structure on $|M|$. The functions $g(z)$ can be used as patching functions for a line bundle S such that $S \otimes_{\mathbb{C}} S = T|M|$. As explained before, a complex structure on a two-dimensional manifold corresponds to a conformal class of metrics $[g]$. It can be shown that complex line bundles S such that $S \otimes_{\mathbb{C}} S = T|M|$ are spinor bundles associated to a spin structure to any metric g in the conformal class. □

The Proposition 2.3 shows that super Riemann surfaces over $\mathbb{R}^{0|0}$ are in one to one correspondence to Riemann surfaces with spinor bundles. For non-trivial families of super Riemann surfaces $M \to B$ the proof of Proposition 2.3 fails because the change of variables formula (6) can get more complicated in the presence of odd dimensions in the base B (see [4]). We will see below that the additional information of a spinor valued differential form χ is needed to describe non-trivial families of super Riemann surfaces.

It was furthermore shown in [19, 24, Theorem 8.4.4] that there is a semi-universal family $\mathcal{E} \to \mathcal{ST}_p$ of super Riemann surfaces of genus p. That is any family $M \to B$ of super Riemann surfaces can be obtained in a non-unique way as a pullback of $\mathcal{E}$ along a map $B \to \mathcal{ST}_p$. The base manifold $\mathcal{ST}_p$ is a super manifold over $\mathbb{R}^{0|0}$ of real dimension $6p - 6|4p - 4$. Proposition 2.3 proves that the points of $|\mathcal{ST}_p|$, i.e. maps $\mathbb{R}^{0|0} \to \mathcal{ST}_p$, are in one to one correspondence to Riemann surfaces with a chosen spinor bundle. The super structure of $\mathcal{ST}_p$ is encoded in non-trivial families of super Riemann surfaces. In order to study non-trivial families of super Riemann surfaces we will turn to a more differential geometric description of super Riemann surfaces:

Theorem 2.4 ([11]) *A super Riemann surface is a* $2|2$*-dimensional real super manifold with a reduction of the structure group of its frame bundle to*

$$G = \left\{ \begin{pmatrix} A^2 & B \\ 0 & A \end{pmatrix} \middle| A, B \in \mathbb{C} \right\} \subset \mathrm{GL}_{\mathbb{C}}(1|1) \subset \mathrm{GL}_{\mathbb{R}}(2|2)$$

together with suitable integrability conditions. Remember that $\mathbb{C}$ *is to be understood as the trivial family* $\mathbb{C} \times B$.

Theorem 2.4 is also interesting for the physical motivation of super Riemann surfaces. It was shown in [11] that the integrability conditions of Theorem 2.4 are related to the so-called "Torsion-constraints" that can be found in more physics-oriented papers as [7, 8]. For a more recent approach via connections on super manifolds and their torsion consult [18, 21].

The Theorem 2.4 shows that it is impossible to describe the geometry of super Riemann surfaces as a super conformal class of super metrics. Any orthogonal matrix that is upper triangular would indeed be diagonal. Consequently $\mathrm{O}(2|2) \not\subseteq G$, i.e. the choice of a super metric is not sufficient to determine a super Riemann surfaces. However there are particular super metrics that are compatible with the structure of a super Riemann surface. They are given by further reduction to U(1) as follows

$$\begin{aligned} \mathrm{U}(1) &\to G \\ U &\mapsto \begin{pmatrix} U^2 & 0 \\ 0 & U \end{pmatrix}. \end{aligned}$$

A further reduction of the structure group to U(1) as above leads to a splitting of the following short exact sequence:

$$0 \longrightarrow \mathcal{D} \longrightarrow TM = \mathcal{D}^{\perp} \oplus \mathcal{D} \underset{p}{\longrightarrow} TM/\mathcal{D} \longrightarrow 0 \tag{7}$$

Consider now an embedding of an underlying even manifold $i\colon |M| \to M$ for a fixed super Riemann surface M. Recall that the underlying even manifold $|M|$ of the super manifold M is a family of super manifolds of relative dimension $2|0$ over the base B. The pullback of the short exact sequence (7) along an embedding i

$$0 \longrightarrow S \longrightarrow i^*TM \underset{Ti}{\overset{\tilde{p}}{\rightleftarrows}} T|M| \longrightarrow 0$$

possesses a second splitting given by Ti. By the identification $T|M| = i^*\mathcal{D}^{\perp}$, the tangent bundle of $|M|$ gets equipped with a metric g. The bundle $S = i^*\mathcal{D}$ is a spinor bundle of the metric g because $i^*\mathcal{D} \otimes_{\mathbb{C}} i^*\mathcal{D} = i^*TM/\mathcal{D} = T|M|$.

The difference of the splittings $\tilde{p}$ and Ti is a section of $T^{\vee}|M| \otimes S$ which we call gravitino χ.

$$\chi(v) = p_S\,(\tilde{p} - Ti)\,v.$$

Here $p_S\colon i^*TM \to S$ is the projector given by the splitting of the short exact sequence by $\tilde{p}$.

The construction given here associates to any super Riemann surface M with additional U(1)-structure a triple (g, S, χ) that consists of a metric g, a spinor bundle S and a gravitino field χ on the underlying surface $|M|$. Different choices of U(1)-structure on the same super Riemann surface lead to metrics and gravitinos which differ from g and χ only by a conformal and super Weyl transformation. A super Weyl transformation is a transformation of the gravitino given by

$$\chi(v) \mapsto \chi(v) + \gamma(v)t$$

Here t is a section of S and $\gamma: T|M| \to \mathrm{End}(S)$ is Clifford multiplication and v a tangent vector field to $|M|$.

It is surprising that the metric g, the spinor bundle S and the gravitino χ contain full information about the super Riemann surface M. Indeed, it was shown in [16] that the super Riemann surface M and the embedding $i: |M| \to M$ can be reconstructed from the metric, the spinor bundle and the gravitino. Thus there is a bijection

$$\{i: |M| \to M, M \text{ super Riemann surface}\} \longleftrightarrow \{|M|, S, g, \chi\} \,/\text{Weyl, SWeyl.}$$

The metric g and the gravitino χ do explicitly depend on the embedding i. The normal bundle to the embedding $i: |M| \to M$ is $S = i^*\mathcal{D}$. Thus an infinitesimal deformation of the embedding i is given by a section q of S. The resulting infinitesimal change of metric and gravitino is given by (c.f. [16]):

$$\begin{aligned} \delta f_a &= -2\langle \gamma^b q, \chi(f_a)\rangle f_b \\ \delta\chi_a &= \nabla^S_{f_a} q = \nabla^{LC}_{f_a} q + \langle \gamma^b \chi_b, \chi_a\rangle \gamma^1\gamma^2 q \end{aligned} \tag{8}$$

Here the metric is expressed in terms of an orthonormal frame f_a and the gravitino in components $\chi_a = \chi(f_a)$. The spinor covariant derivative ∇^{LC} is the Levi-Civita connection lifted to S. Equations (8) are known as super symmetry transformations of the metric and gravitino and will be a symmetry of the action functional $A(\varphi, g, \psi, \chi, F)$ below. Furthermore one can show that it is possible to choose an embedding i such that the gravitino vanishes around a given point $p \in |M|$. If M is a trivial family of super Riemann surfaces it is possible to choose an embedding i such that the gravitino vanishes on the whole of $|M|$.

Having a description of super Riemann surfaces in terms of metrics and gravitinos, it is natural to ask for a description of the super moduli space in terms of metrics and gravitinos. Conjectures about such a super Teichmüller space can be found in the literature, see e.g. [8, 15, Equation 3.85]. It is expected that there is a one-to-one correspondence

$$\{M, M \text{ super Riemann surface}\} \,/\, \mathrm{SDiff}(M)$$

$$\longleftrightarrow$$

$$\{|M|, S, g, \chi\} \,/ \mathrm{Weyl}, \mathrm{SWeyl}, \mathrm{Diff}(|M|), \mathrm{SUSY} \tag{9}$$

The group of super symmetry transformations SUSY on the right hand side can probably be identified with the change of embedding i. A precise definition of SUSY and the study of the full quotient must be left for further research. A particularly interesting question is, how the quotient by SUSY is related to the nonprojectedness of the super moduli space (see [9]).

However it is possible to study an infinitesimal version of the quotient (9). That is infinitesimal deformations of super Riemann surfaces can be studied in terms of infinitesimal deformations of metrics and gravitino. Similar to Eq. (5) it is possible to decompose the infinitesimal deformations

$$\delta g = \lambda g + L_X g + \mathrm{susy}(q) + D$$
$$\delta \chi = \gamma t + L_X \chi + \mathrm{susy}(q) + \mathfrak{D}$$

Here $\mathrm{susy}(q)$ denotes the infinitesimal super symmetry transformations from Eq. (8). λg is the infinitesimal Weyl transformation and γt the infinitesimal super Weyl transformation. It is possible to determine the free parameters λ, t, X, and q such that the remaining "true deformations" D and $\mathfrak{D}$ are holomorphic sections of $T^\vee|M| \otimes_{\mathbb{C}} T^\vee|M|$ and $S^\vee \otimes_{\mathbb{C}} S^\vee \otimes_{\mathbb{C}} S^\vee$ respectively. More precisely one has the following:

Theorem 2.5 ([16]) *Let M be the super Riemann surface given by g, S and χ under the embedding $i\colon |M| \to M$. The infinitesimal deformations of M are given by*

$$H^0(T^\vee|M| \otimes_{\mathbb{C}} T^\vee|M|) \oplus H^0(S^\vee \otimes_{\mathbb{C}} S^\vee \otimes_{\mathbb{C}} S^\vee)$$

Here H^0 denotes holomorphic sections.

This result is well-known (see e.g. [24] and references therein). However, the approach outlined here gives a much more geometrical description of the even and odd infinitesimal deformations as infinitesimal deformations of the metric and gravitino, respectively.

3 Action Functional

In this chapter we are investigating a super symmetric extension of the harmonic action functional on Riemann surfaces. This non-linear super symmetric sigma model can be formulated as an integral over a super Riemann surface and may help,

like the harmonic action functional on Riemann surfaces, to understand the moduli space of super Riemann surfaces.

Let us first recall how the harmonic action functional on Riemann surfaces can be used as a tool to study the Teichmüller space. Details can be found in [13, 14]. Let $\varphi\colon |M| \to N$ be a smooth map from the Riemann surface $(|M|, g)$ to the Riemannian manifold (N, n). The harmonic action functional as a functional of the metric g and the map φ is given by

$$A(g,\varphi) = \int_{|M|} \| d\varphi \|^2_{g^\vee \otimes \varphi^* n} \, dvol_g \tag{10}$$

The maps φ which are critical points of $A(g,\varphi)$ are called harmonic maps.

In the case of two dimensional domains, as considered here, the action is conformally invariant, i.e. $A(\Lambda g, \varphi) = A(g,\varphi)$. The action functional $A(g,\varphi)$ can thus be considered as a functional on the conformal class of metrics. Furthermore it is diffeomorphism invariant, i.e. for any diffeomorphism $f\colon |M| \to |M|$

$$A(f^* g, \varphi \circ f) = A(g,\varphi)$$

The harmonic action functional can thus be viewed as a functional on isomorphism classes of Riemann surfaces in the sense of Eq. (3) and also on the Teichmüller space, see Eq. (4).

Define the energy-momentum tensor as the variation of $A(g,\varphi)$ with respect to the metric g:

$$\delta_g A(g,\varphi) = \int_{|M|} \delta g \cdot T \, dvol_g \tag{11}$$

For a harmonic map φ the energy-momentum-tensor is the Noether current that corresponds to diffeomorphism invariance. Infinitesimal conformal rescalings $\delta g = \lambda g$ and Lie-derivatives $\delta g = L_X g$ must lie in the kernel of the variation $\delta_g A$. The vanishing of $\delta_g A$ on infinitesimal conformal rescalings and Lie-derivatives is sufficient to show that the energy-momentum tensor T can be identified with a holomorphic quadratic differential.

The preceding facts are particularly interesting in the case where the codomain (N, n) is also a Riemann surface. Let us assume that the genus of Riemann surfaces $|M|$ and N is strictly larger than one. It is possible to assume that the metrics g and n have constant curvature -1. If, furthermore, the Riemann surfaces $(|M|, g)$ and (N, n) are of the same genus p there is a unique harmonic map $\varphi\colon |M| \to N$ homotopic to the identity (see [14, Corollary 3.10.1]). The energy-momentum-tensor T gives a map

$$\mathcal{T}_p \to \Gamma_{|M|}(T^\vee |M| \otimes_{\mathbb{C}} T^\vee |M|) \tag{12}$$

sending the Riemann surface (N, n) to the holomorphic quadratic differential T associated to φ. The Teichmüller theorem [14, Thm 4.2.2] states that the above map (12) is a diffeomorphism. The theorem of Riemann-Roch shows that the right-hand side of (12), is a finite-dimensional vector space isomorphic to $\mathbb{C}^{3p-3} \simeq \mathbb{R}^{6p-6}$.

Summing up, we have seen that the harmonic action functional and harmonic maps help to prove fundamental results in the theory of Teichmüller space. Furthermore, as is shown in [13], harmonic maps are also useful to study a quantized version of the harmonic action functional. We now present the outline of a similar theory in the case of super Riemann surfaces.

Let M be a super Riemann surface with a fixed U(1)-structure and local U(1)-frames F_A. Let $\Phi: M \to N$ be a map to an arbitrary Riemannian (super) manifold (N, n). The super symmetric extension of the harmonic action functional (10) is given by

$$A(M, \Phi) = \int_M \| \, d\Phi|_{\mathcal{D}} \, \|^2 [dvol] = \int_M \varepsilon^{\alpha\beta} \langle F_\alpha \Phi, F_\beta \Phi \rangle_{\Phi^* n} [F^1 F^2 F^3 F^4] \tag{13}$$

At a first glance this action functional looks just like the harmonic action functional (10). However notice that the norm of the differential $d\Phi$ restricted to $\mathcal{D}$ is used. This difference to the harmonic action functional is crucial to show that the action functional ((13)) does only depend on the underlying G-structure and not on the chosen U(1)-structure. This analogue of conformal invariance, together with the super diffeomorphism invariance of $A(M, \Phi)$ turns $A(M, \Phi)$ into a functional on the moduli space of super Riemann surfaces as in the left-hand side of Eq. (9).

The action functional ((13)) can be found at different places in the literature, see for example [8, 11]. In [11] the super conformal invariance of the action functional $A(M, \Phi)$ is shown.

The maps Φ that are critical with respect to $A(M, \Phi)$ are described by a differential equation of second order:

$$0 = \Delta^{\mathcal{D}} \Phi = \varepsilon^{\alpha\beta} \nabla_{F_\alpha} F_\beta \Phi + \varepsilon^{\alpha\beta} \, (\operatorname{div} F_\alpha) \, F_\beta \Phi \tag{14}$$

Analytical properties of the $\mathcal{D}$-Laplace operator $\Delta^{\mathcal{D}}$, defined here, still need to be studied. Remember that a detailed understanding of the analysis of harmonic maps is crucial for the definition of the Teichmüller map (12). In [16] it was shown that Eq. (14) can be used to derive equations of motion for the component fields defined below in Definition 3.1.

Let now $i: |M| \to M$ be an underlying even manifold for M. We have seen in the last section that the super Riemann surface M can be described in terms of a metric field g and a gravitino field χ. As explained in the first section, every integral over a super manifold can be reduced to an integral over the underlying even manifold. Let us denote the resulting Lagrangian density on $|M|$ by $|L|$, i.e.:

$$A(M, \Phi) = \int_{|M|} |L|$$

Of course the Lagrangian density $|L|$ depends not only on g and χ, but also on Φ. In order to express this dependence in a geometric way, we will now introduce component fields for Φ.

Definition 3.1 Let $\Phi: M \to N$ be a morphism and $i: |M| \to M$ be an underlying even manifold. We call the fields

$$\begin{array}{lll} \varphi: |M| \to N & \psi: |M| \to S^\vee \otimes \varphi^* TN & F: |M| \to \varphi^* TN \\ \varphi = \Phi \circ i & \psi = s^\alpha \otimes i^* F_\alpha \Phi & F = i^* \Delta^{\mathcal{D}} \Phi \end{array}$$

component fields of Φ. The vectors s^α form the dual basis to the basis $s_\alpha = i^* F_\alpha$ of the spinor bundle $S = i^* \mathcal{D}$ on $|M|$.

The component fields are sufficient to fully determine the map Φ. There are particular coordinates (x^a, η^α) on M such that in the case $N = \mathbb{R}$ the map Φ can be written as

$$\Phi^\# r = \varphi + \eta^\mu \psi_\mu + \eta^1 \eta^2 F$$

This expansion is similar to the Example 1.8. It is an advantage of the geometric definition of the component fields φ, ψ and F, used here, to apply for arbitrary target manifolds N.

With the help of the component maps φ, ψ and F, as well as g and χ, the Lagrangian density $|L|$ can be calculated explicitly. For details on the rather long computations, see the forthcoming thesis [17]. Note that the reduction of the action functional $A(M, \Phi)$ to the action functional $A(\varphi, g, \psi, \chi, F)$ given below was claimed in the literature almost 30 years ago (see, for example, [8]). This reduction served as a major motivation for the introduction of super Riemann surfaces, as supposedly the action functional $A(M, \Phi)$ would be easier to study than the component action $A(\varphi, g, \psi, \chi, F)$. However, no proof of the reduction could be found in the literature.

Theorem 3.2 *Let M be a super Riemann surface and $i: |M| \to M$ an underlying even manifold. We denote by g, χ, and g_S respectively the metric, gravitino, and spinor metric on $|M|$ induced by a given* $\mathrm{U}(1)$*-structure on M. Let $\Phi: M \to N$ be a morphism to a super Riemannian manifold (N, n) and φ, ψ, and F its component fields, as introduced in Definition 3.1. One obtains*

$$\begin{aligned} A(M, \Phi) = A(\varphi, g, \psi, \chi, F) = \int_{|M|} \| d\varphi \|^2_{g^\vee \otimes \varphi^* n} + \langle \psi, \not{D} \psi \rangle_{g_S^\vee \otimes \varphi^* n} \\ - \frac{1}{4} \langle F, F \rangle_{\varphi^* n} + 2 \langle \gamma^a \gamma^b \chi_a \partial_{x^b} \varphi, \psi \rangle_{g_S^\vee \otimes \varphi^* n} + \frac{1}{2} \langle \chi_a, \gamma^b \gamma^a \chi_b \rangle_{g_S} \langle \psi, \psi \rangle_{g_S^\vee \otimes \varphi^* n} \\ + \frac{1}{6} \varepsilon^{\alpha\beta} \varepsilon^{\gamma\delta} \langle R^{\varphi^* TN}(\psi_\alpha, \psi_\gamma) \psi_\delta, \psi_\beta \rangle_{\varphi^* n} \, dvol_g \end{aligned}$$

Notice that the symmetries of $A(M,\Phi)$ translate into several symmetries for $A(\varphi,g,\psi,\chi,F)$. The G-invariance of the action $A(M,\Phi)$ leads to conformal and super Weyl invariance of $A(\varphi,g,\psi,\chi,F)$. The invariance of $A(M,\Phi)$ under super diffeomorphisms splits into diffeomorphism invariance and super symmetry of $A(\varphi,g,\psi,\chi,F)$. Super symmetry of $A(\varphi,g,\psi,\chi,F)$ is the invariance up to first order under an infinitesimal change of the embedding i parametrized by the spinor q. The formulas for the super symmetry between g and χ have been given in Eq. (8). A full calculation for the super symmetry of φ, ψ and F can be found in [17]. We give here the resulting formulas for the special case $F=0$ and $R^N=0$:

$$\delta\varphi = \langle q,\psi\rangle \qquad\qquad \delta\psi = \left(\partial_{x^k}\varphi - \langle\psi,\chi_k\rangle\right)\gamma^k q$$

We have thus given a super geometric explanation to all symmetries of the action functional $A(\varphi,g,\psi,\chi,F)$ appearing in the literature (e.g. [2, 7]).

We now turn to applications of the action functional $A(M,\Phi)$ to the super moduli space or super Teichmüller space. Similar to the case of Riemann surfaces and the harmonic action functional, the action functional $A(M,\Phi)$ can be seen as a functional on the super moduli space. By the left hand side of Eq. (9) the super moduli space is given by the integrable G-structures up to super diffeomorphisms. The action functional ((13)) depends explicitly on the G-structure and is super diffeomorphism invariant. Thus one may expect that the action functional (13) and its critical points—the maps $\Phi: M \to N$ solving Eq. (14)—may be useful to study the super moduli space. However certain difficulties arise from the presence of integrability conditions in Theorem 2.4. Let H be an infinitesimal variation of the G-frame F_A, i.e. first derivative of a family of frames

$$F(t)_A = F_A + tH_A^B F_B + o(t).$$

If the family of frames $F(t)_A$ is a family of integrable G-frames, certain infinitesimal integrability conditions hold for H. Consequently, the H that do not fulfil those infinitesimal integrability conditions are not admissible infinitesimal deformations of the super Riemann surface defined by F_A.

The variation of the action functional ((13)) with respect to the variation of the frames F_A can be written as

$$\delta_{F_A} A(M,\Phi) = \int_M H \cdot T^{super}[dvol] \tag{15}$$

The tensor T^{super} can be seen as a super version of the energy-momentum-tensor in Eq. (11). However it is not guaranteed that non-integrable infinitesimal deformations H lie in the kernel of the variation $\delta_{F_A} A(M,\Phi)$. Thus, in contrast to the case of Riemann surfaces, $\delta_{F_A} A(M,\Phi)$ can not be interpreted as a cotangent vector to the moduli space of super Riemann surfaces.

In order to circumvent the problem of integrability conditions one can turn to a description of the moduli space of super Riemann surfaces in terms of metrics and

gravitinos, i.e. to the right hand side of Eq. (9). It is an advantage of the description of super Riemann surfaces in terms of metrics and gravitinos that there are no integrability conditions, i.e. every triple (g, S, χ) forms a super Riemann surface. Thus every deformation of the given metric and given gravitino is an admissible deformation of the super Riemann surface at hand. Define the energy-momentum tensor T of $A(\varphi, g, \psi, \chi, F)$ via

$$\delta_g A(\varphi, g, \psi, \chi, F) = \int_{|M|} \delta g \cdot T \, dvol_g$$

and the super current J by

$$\delta_\chi A(\varphi, g, \psi, \chi, F) = \int_{|M|} \delta\chi \cdot J \, dvol_g$$

If the fields φ, ψ, and F are critical points of $A(\varphi, g, \psi, \chi, F)$, then T is the Noether current with respect to diffeomorphism invariance, whereas J is the Noether current with respect to super symmetry. It can be shown that T and J are components of T^{super} similar to φ, ψ and F being components of Φ. Thus, once again, diffeomorphism invariance and super symmetry are very much the same thing from the viewpoint of super geometry. With the help of the diffeomorphism invariance and super symmetry of $A(\varphi, g, \psi, \chi, F)$ one can show that T is, once again, a holomorphic quadratic differential and J a holomorphic section of $S^\vee \otimes_{\mathbb{C}} S^\vee \otimes_{\mathbb{C}} S^\vee$. They are even, resp. odd tangent vectors to the moduli space of super Riemann surfaces.

One can hope that the study of critical points of the action functional $A(\varphi, g, \psi, \chi, F)$ turns out as useful for the study of the moduli space of super Riemann surfaces as the study of harmonic maps is for Teichmüller theory.

Acknowledgements I want to thank the organizers of the conference "Quantum Mathematical Physics", Felix Finster, Jürgen Tolksdorf, and Eberhard Zeidler for inviting me to this most inspiring conference and for the opportunity to present my research.

The research leading to these results has received funding from the European Research Council under the European Union's Seventh Framework Programme (FP7/2007–2013)/ERC grant agreement no. 267087. The research has been carried out at the Max-Planck-Institut für Mathematik in den Naturwissenschaften as a student of the International Max Planck Research School Mathematics in the Sciences. I am grateful for the support received.

References

1. M. Batchelor, Two approaches to supermanifolds. Trans. Am. Math. Soc. **258**(1) (1980). doi:10.1090/S0002-9947-1980-0554332-9
2. L. Brink, P. di Vecchia, P. Howe, A locally supersymmetric and reparametrization invariant action for the spinning string. Phys. Lett. B **65**(5), 471–474 (1976). doi:10.1016/0370-2693(76)90445-7

3. C. Carmeli, L. Caston, R. Fioresi, *Mathematical Foundations of Supersymmetry* (European Mathematical Society, Zürich, 2011). doi:10.4171/097
4. L. Crane, J.M. Rabin, Super Riemann surfaces: uniformization and Teichmüller theory. Commun. Math. Phys. **113**(4), 601–623 (1988). doi:10.1007/BF01223239
5. P. Deligne, D.S. Freed, Supersolutions, in *Quantum Fields and Strings: A Course for Mathematicians*, vol. 1, ed. by P. Deligne et al., 2 vols. (American Mathematical Society, Providence, 1999), pp. 227–356. arXiv:hep-th/9901094. http://www.math.ias.edu/qft (visited on 19 Jan 2015)
6. P. Deligne, J.W. Morgan, Notes on supersymmetry (following Joseph Bernstein), in *Quantum Fields and Strings: A Course for Mathematicians*, vol. 1, ed. by P. Deligne et al., 2 vols. (American Mathematical Society, Providence, 1999), pp. 41–98. http://www.math.ias.edu/qft (visited on 19 Jan 2015)
7. S. Deser, B. Zumino, A complete action for the spinning string. Phys. Lett. B **65**(4), 369–373 (1976). doi:10.1016/0370-2693(76)90245-8
8. E. D'Hoker, D.H. Phong, The geometry of string perturbation theory. Rev. Mod. Phys. **60**(4), 917–1065 (1988). doi:10.1103/RevModPhys.60.917
9. R. Donagi, E. Witten, *Supermoduli Space Is Not Projected* (2013, pre-published) arXiv:1304.7798 [hep-th]
10. D. Friedan, Notes on string theory and two dimensional conformal field theory, in *Unified String Theories*. Proceedings. Workshop on Unified String Theories (Institute for Theoretical Physics, Santa Barbara, July 29–Aug 16, 1985). ed. by M.B. Green, D.J. Gross (World Scientific, Singapore, 1986), pp. 162–213
11. S.B. Giddings, P. Nelson, The geometry of super Riemann surfaces. Commun. Math. Phys. **116**(4), 607–634 (1988). doi:10.1007/BF01224903
12. A. Grothendieck, J. Dieudonné, Éléments de géometrie algébrique. I. Le langage des schémas. French. Publ. Math. IHÉS **4**, 5–228 (1960). http://www.numdam.org/item?id=PMIHES_196__4__5_0 (visited on 2 Mar 2015)
13. J. Jost, *Bosonic Strings. A Mathematical Treatment*. Studies in Advanced Mathematics, vol. 21 (American Mathematical Society/International Press, Cambridge, 2001), 95pp.
14. J. Jost, *Compact Riemann Surfaces*. An Introduction to Contemporary Mathematics, 3rd edn. Universitext (Springer, Berlin, 2006), pp. xviii + 277. doi:10.1007/978-3-540-33067-7
15. J. Jost, *Geometry and Physics* (Springer, Berlin, 2009), pp. xiv + 217. doi:10.1007/978-3-642-00541-1
16. J. Jost, E. Keßler, J. Tolksdorf, *Super Riemann Surfaces, Metrics, and the Gravitino* (2014, submitted). arXiv:1412.5146 [math-ph]
17. E. Keßler, PhD thesis. Universität Leipzig (2015, in preparation)
18. E. Keßler, *U*(1)*-connections on Super Riemann Surfaces* (2015, in preparation)
19. C. LeBrun, M. Rothstein, Moduli of super Riemann surfaces. Commun. Math. Phys. **117**(1), 159–176 (1988). doi:10.1007/BF01228415
20. D.A. Leites, Introduction to the theory of supermanifolds. Russ. Math. Surv. **35**(1), 1–64 (1980). doi:10.1070/RM1980v035n01ABEH001545
21. J. Lott, Torsion constraints in supergeometry. Commun. Math. Phys. **133**(3), 563–615 (1990). doi:10.1007/BF02097010
22. Y.I. Manin, Critical dimensions of the string theories and the dualizing sheaf on the moduli space of (super) curves. Funct. Anal. Appl. **20**(3), 244–246 (1986). doi:10.1007/BF01078480
23. A. Rogers, A global theory of supermanifolds. J. Math. Phys. **21**(6), 1352–1365 (1980). doi:10.1063/1.524585
24. C. Sachse, Global analytic approach to super Teichmüller Spaces, PhD thesis. Universität Leipzig, 19 Feb 2009. arXiv:0902.3289 [math.AG]

Recent Developments in Deformation Quantization

Stefan Waldmann

Contents

Abstract In this review an overview on some recent developments in deformation quantization is given. After a general historical overview we motivate the basic definitions of star products and their equivalences both from a mathematical and a physical point of view. Then we focus on two topics: the Morita classification of star product algebras and convergence issues which lead to the nuclear Weyl algebra.

Keywords Star products • Deformation quantization • Morita classification • Weyl algebra

Mathematics Subject Classification (2010). Primary 53D55; Secondary 16D90, 46H05, 46K05, 46A03

S. Waldmann (✉)
Institut für Mathematik, Universität Würzburg, Campus Hubland Nord, Emil-Fischer-Straße 31, 97074 Würzburg, Germany
e-mail: stefan.waldmann@mathematik.uni-wuerzburg.de

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_18

1 Introduction: A Historical Tour d'Horizon

In the last decades, deformation quantization evolved into a widely accepted quantization scheme which, on one hand, provides deep conceptual insights into the question of quantization and, on the other hand, proved to be a reliably technique leading to explicit understanding of many examples. It will be the aim of this review to give some overview on the developments of deformation quantization starting from the beginnings but also including some more recent ideas.

The original formulations of deformation quantization by Bayen et. al. aimed mainly at finite-dimensional classical mechanical systems described by symplectic or Poisson manifolds [5] and axiomatized the heuristic quantization formulas found earlier by Weyl, Groenewold and Moyal [56, 73, 89]. Berezin considered the more particular case of bounded domains and Kähler manifolds [7–9]. Shortly after it proved to be a valuable tool to approach also problems in quantum field theories, see e.g. the early works of Dito [41–43].

Meanwhile, the question of existence and classification of deformation quantizations, i.e. of star products, on symplectic manifolds was settled: first DeWilde and Lecomte showed the existence of star products on symplectic manifolds [39] in 1983 after more particular classes [38, 40] had been considered. Remarkably, also in 1983 the first genuine class of Poisson structures was shown to admit star products, the linear Poisson structures on the dual of a Lie algebra, by Gutt [57] and Drinfel'd [47]. In 1986 Fedosov gave a very explicit and constructive way to obtain star products on a symplectic manifold by means of a symplectic connection [53], see also [54, 55] for a more detailed version. His construction is still one of the cornerstones in deformation quantization as it provides not only a particularly nice construction allowing to adjust many special features of star products depending on the underlying manifold like e.g. separation of variables (Wick type) on Kähler manifolds [14, 61, 62, 79] or star products on cotangent bundles [19–21]. Even beyond the symplectic world, Fedosov's construction was used to globalize the existence proofs of star products on Poisson manifolds [36, 44].

Even though the symplectic case was understood well, the question of existence on Poisson manifolds kept its secrets till the advent of Kontsevich's formality theorem, solving his formality conjecture [63, 64, 67]. To give an adequate overview on Kontsevich's formality theorem would clearly go beyond the scope of this short review. Here one can rely on various other publications like e.g. [35, 52]. In a nutshell, the formality theorem proves a very general fact about smooth functions on a manifold from which it follows that every (formal series of) Poisson structures can be quantized into a star product, including a classification of star products. Parallel to Kontsevich's groundbreaking result, the classification of star products on symplectic manifolds was achieved and compared by several groups [10, 37, 58, 77, 78]. Shortly after Kontsevich, Tamarkin gave yet another approach to the quantization problem on Poisson manifolds [84], see also [65, 68], based on the language of operads and the usage of Drinfel'd associators. Starting with these formulations, formality

theory has evolved and entered large areas of contemporary mathematics, see e.g. [1–3, 45, 46, 65, 66] to name just a few.

While deformation quantization undoubtedly gave many important contribution to pure mathematics over the last decades, it is now increasingly used in contemporary quantum physics as well: perhaps starting with the works of Dütsch and Fredenhagen on the perturbative formulations of algebraic quantum field theory [49–51] it became clear that star products provide the right tool to formulate quantum field theories in a semiclassical way, i.e. as formal power series in $\hbar$. Now this has been done in increasing generalities for various scenarios including field theories on general globally hyperbolic spacetimes, see e.g. [4, 22, 23, 59].

Of course, from a physical point of view, deformation quantization can not yet be the final answer as one always deals with formal power series in the deformation parameter $\hbar$. A physically reasonable quantum theory, however, requires of course convergence. Again, in the very early works [5] some special cases were treated, namely the Weyl-Moyal product for which an integral formula exists which allows for a reasonable analysis based on the Schwartz space. The aims here are at least two-fold. On one hand one wants to establish a reasonable spectral calculus for particular elements in the star product algebra which allows to compute spectra in a physically sensitive way. This can be done with the star exponential formalism, which works in particular examples but lacks a general framework. On the other hand, one can try to establish form the formal star product a convergent version such that in the end one obtains a C^*-algebra of quantum observables being a deformation, now in a continuous way, of the classical functions on the phase space. This is the point of view taken by strict deformation quantization, most notably advocated by Rieffel [81, 82] and Landsman [70], see also [16, 30–33] for the particular case of quantizable Kähler manifolds and [74–76] for more general symplectic manifolds. Bieliavsky and coworkers found a generalization of Rieffel's approach by passing from actions of the abelian group $\mathbb{R}^d$ to more general Lie group actions [11–13]. Having a C^*-algebra one has then the full power of C^*-algebra techniques at hands which easily allows to get a reasonable spectral calculus. However, constructing C^*-algebraic quantizations is still very much in development: here one has not yet a clear picture on the existence and classification of the quantizations. In fact, one even has several competing definitions of what one is looking for. It is one of the ongoing research projects by several groups to understand the transition between formal and strict quantizations in more detail.

Needless to say, in the above historical survey we can barely scratch on the surface of this vast topic: many aspects have not been mentioned like the role played of symmetries and reduction, the applications to concrete physical systems, various generalizations of deformation quantization to other geometric brackets, relations to noncommutative geometry, and many more. In the remaining part of this review we will focus on two aspects of the theory: first, we discuss the role of classification results beyond the notion of equivalence, i.e. isomorphism. Here we are particularly interested in the classification of star products up to Morita equivalence. Second, we give a short outlook on star products in infinite dimensions and problems arising there by investigating one particular example: the Weyl algebra of a vector space

with a (quite arbitrary) bilinear form. Beside the purely algebraic construction we obtain a locally convex algebraic deformation once we start in this category.

2 From Poisson Manifolds to Star Products

In this section we give a more detailed but still non-technical motivation of the definition of star products and list some first examples.

The set-up will be a finite-dimensional phase space which we model by a symplectic or, more generally, a Poisson manifold (M, π) where $\pi \in \Gamma^\infty(\Lambda^2 TM)$ is a bivector field satisfying

$$[\![\pi, \pi]\!] = 0. \tag{1}$$

Here $[\![\cdot, \cdot]\!]$ is the Schouten bracket and the condition is equivalent to the Jacobi identity for the Poisson bracket

$$\{f, g\} = -[\![[\![f, \pi]\!], g]\!] = \pi(\mathrm{d}f, \mathrm{d}g) \tag{2}$$

determined by π for functions $f, g \in \mathscr{C}^\infty(M)$. One can then formulate classical Hamiltonian mechanics using π and $\{\cdot, \cdot\}$. For a gentle introduction to Poisson geometry see [87] as well as [34, 48, 71, 85]. There are several important examples of Poisson manifolds:

- Every symplectic manifold (M, ω), where $\omega \in \Gamma^\infty(\Lambda^2 T^*M)$ is a closed non-degenerate two-form, is a Poisson manifold with $\pi = \omega^{-1}$. The Jacobi identity (1) corresponds then directly to $\mathrm{d}\omega = 0$.
- Every cotangent bundle T^*Q is a symplectic manifold in a canonical way with an exact symplectic form $\omega = \mathrm{d}\theta$ where $\theta \in \Gamma^\infty(T^*(T^*Q))$ is the canonical (or tautological) one-form on T^*Q.
- Kähler manifolds are particularly nice examples of symplectic manifolds as they possess a compatible Riemannian metric and a compatible complex structure.
- The dual $\mathfrak{g}^*$ of a Lie algebra $\mathfrak{g}$ is always a Poisson manifold with a linear Poisson structure: the coefficient functions of the tensor field π are linear functions on $\mathfrak{g}^*$, explicitly given by

$$\{f, g\}(x) = x_i c^i_{k\ell} \frac{\partial f}{\partial x^k} \frac{\partial g}{\partial x^\ell}, \tag{3}$$

  where $x_1, \ldots, x_n$ are the linear coordinates on $\mathfrak{g}^*$ and $c^i_{k\ell}$ are the corresponding structure constants of $\mathfrak{g}$. Since (3) vanishes at the origin, this is never symplectic.
- Remarkably and slightly less trivial is the observation that on every manifold M, for every $p \in M$ there is a Poisson structure π with compact support where $\pi\big|_p$ has maximal rank.

To motivate the definition of a star product we consider the most easy example of the classical phase space $\mathbb{R}^2$ with canonical coordinates (q, p). Canonical quantization says that we have to map the spacial coordinate q to the position operator Q acting on a suitable domain in $L^2(\mathbb{R}, \mathrm{d}x)$ as multiplication operator. Moreover, we have to assign the momentum coordinate p to the momentum operator $P = -\mathrm{i}\hbar\frac{\partial}{\partial q}$, again defined on a suitable domain. Since we want to ignore functional-analytic questions at the moment, we simply chose $\mathscr{C}_0^\infty(\mathbb{R})$ as common domain for both operators. In a next step we want to quantize polynomials in q and p as well. Here we face the ordering problem as $pq = qp$ but $PQ \neq QP$. One simple choice is the *standard ordering*

$$q^n p^m \;\mapsto\; \varrho_{\mathrm{Std}}(q^n p^m) = Q^n P^m = (-\mathrm{i}\hbar)^m q^n \frac{\partial^m}{\partial q^m} \tag{4}$$

for monomials and its linear extension to all polynomials. More explicitly, this gives

$$\varrho_{\mathrm{Std}}(f) = \sum_{r=0}^{\infty} \frac{1}{r!} \left(\frac{\hbar}{\mathrm{i}}\right)^r \frac{\partial^r f}{\partial p^r}\Big|_{p=0} \frac{\partial^r}{\partial q^r}. \tag{5}$$

Now this formula still makes sense for smooth functions f which are polynomial only in p, i.e. for $f \in \mathscr{C}^\infty(\mathbb{R})[p]$. The main idea of deformation quantization is now to pull-back the operator product: this is possible since the image of ϱ_{Std} is the space of all differential operators with smooth coefficients which therefore is a (noncommutative) algebra. We define the *standard-ordered star product* by

$$f \star_{\mathrm{Std}} g = {\varrho_{\mathrm{Std}}}^{-1}(\varrho_{\mathrm{Std}}(f)\varrho_{\mathrm{Std}}(g)) = \sum_{r=0}^{\infty} \frac{1}{r!} \left(\frac{\hbar}{\mathrm{i}}\right)^r \frac{\partial^r f}{\partial p^r} \frac{\partial^r g}{\partial q^r} \tag{6}$$

for $f, g \in \mathscr{C}^\infty(\mathbb{R})[p]$. While it is clear that $\star_{\mathrm{Std}}$ is an associative product the behaviour with respect to the complex conjugation is bad: we do not get a *-involution $\overline{f \star_{\mathrm{Std}} g} \neq \overline{g} \star_{\mathrm{Std}} \overline{f}$ since

$$\varrho_{\mathrm{Std}}(f)^\dagger = \varrho_{\mathrm{Std}}(N^2 f) \quad \text{with} \quad N = \exp\left(\frac{\hbar}{2\pi}\frac{\partial^2}{\partial q \partial p}\right), \tag{7}$$

as a simple integration by parts shows. We can repair this unpleasant feature by defining the Weyl ordering and the Weyl product by

$$\varrho_{\mathrm{Weyl}}(f) = \varrho_{\mathrm{Std}}(Nf) \quad \text{and} \quad f \star_{\mathrm{Weyl}} g = N^{-1}(Nf \star_{\mathrm{Std}} Ng). \tag{8}$$

Note that N is indeed an invertible operator on $\mathscr{C}^\infty(\mathbb{R})[p]$. Again, $\star_{\mathrm{Weyl}}$ is associative. Then we get

$$\overline{f \star_{\mathrm{Weyl}} g} = \overline{g} \star_{\mathrm{Weyl}} \overline{f} \quad \text{and} \quad \varrho_{\mathrm{Weyl}}(f \star_{\mathrm{Weyl}} g) = \varrho_{\mathrm{Weyl}}(f)\varrho_{\mathrm{Weyl}}(g). \tag{9}$$

For both products we can collect the terms of order $\hbar^r$ which gives

$$f \star g = \sum_{r=0}^{\infty} \hbar^r C_r(f,g) \tag{10}$$

with bidifferential operators C_r of order r in each argument. The explicit formula for $\star_{\text{Weyl}}$ is slightly more complicated than the one for $\star_{\text{Std}}$ in (6) and easily computed. We have

$$f \star g = fg + \cdots \quad \text{and} \quad f \star g - g \star f = \mathrm{i}\hbar\{f,g\} + \cdots, \tag{11}$$

where $+\cdots$ means higher orders in $\hbar$. Also $f \star 1 = f = 1 \star f$. Note also that the seemingly infinite series in (10) is always finite as long as we take functions in $\mathscr{C}^\infty(\mathbb{R})[p]$.

The idea is now to axiomatize these features for $\star$ in such a way that it makes sense to speak of a star product on a general Poisson manifold. The first obstacle is that on a generic manifold M there is nothing like functions which are polynomial in certain coordinates. This is a chart-dependent characterization which one does not want to use. But then already for $\star_{\text{Weyl}}$ and $\star_{\text{Std}}$ one encounters the problem that for general $f, g \in \mathscr{C}^\infty(\mathbb{R}^2)$ the formulas (6) and (9) will not make any sense: the series are indeed infinite and since we can adjust the Taylor coefficients of a smooth function in a rather nasty way, there is no hope for convergence. The way out is to consider *formal* star product in a first step, i.e. formal power series in $\hbar$. This yields the definition of star products [5]:

Definition 2.1 A formal star product $\star$ on a Poisson manifold (M,π) is an associative $\mathbb{C}[[\hbar]]$-bilinear associative product for $\mathscr{C}^\infty(M)[[\hbar]]$ such that

$$f \star g = \sum_{r=0}^{\infty} \hbar^r C_r(f,g) \tag{12}$$

with

1. $C_0(f,g) = fg$,
2. $C_1(f,g) - C_1(g,f) = \mathrm{i}\{f,g\}$,
3. $C_r(1,f) = 0 = C_r(f,1)$ for $r \geq 1$,
4. C_r is a bidifferential operator.

Already in the trivial example above we have seen that there might be more than one star product. The operator N interpolates between them and is invisible in classical physics: for $\hbar = 0$ the operator N becomes the identity. As a formal series of differential operators it is invertible and implements an algebra isomorphism. This is now taken as definition for equivalence of star products: given two star products $\star$ and $\star'$ on a manifold, a formal power series $T = \sum_{r=0}^{\infty} \hbar^r T_r$ of differential operators T_r with $T1 = 1$ is called an equivalence between $\star$ and $\star'$

if

$$f \star' g = T^{-1}(Tf \star Tg). \tag{13}$$

Note that T is indeed invertible as a formal power series. Hence this is an equivalence relation. Conversely, given such a T and $\star$ we get a new star product $\star'$ by (13).

We list now some basic examples of star products:

- The explicit formulas for $\star_{\text{Std}}$ and $\star_{\text{Weyl}}$ immediately generalize to higher dimensions yielding equivalent star products on $\mathbb{R}^{2n}$ and hence also on every open subset of $\mathbb{R}^{2n}$. Since by the Darboux Theorem every symplectic manifold looks like an open subset of $\mathbb{R}^{2n}$ *locally*, the question of existence of star products on symplectic manifolds is a global problem.
- For the linear Poisson structure (3) on the dual $\mathfrak{g}^*$ of a Lie algebra $\mathfrak{g}$ one gets a star product as follows [57]: First, we note that the symmetric algebra $\mathrm{S}^\bullet(\mathfrak{g})$ over $\mathfrak{g}$ can be canonically identified with the polynomials $\mathrm{Pol}^\bullet(\mathfrak{g}^*)$ on the dual $\mathfrak{g}^*$. Then the PBW isomorphism

$$\mathrm{S}^\bullet(\mathfrak{g}) \ni \xi_1 \vee \cdots \vee \xi_k \;\mapsto\; \frac{(\mathrm{i}\hbar)^k}{k!} \sum_{\sigma \in S_k} \xi_{\sigma(1)} \cdots \xi_{\sigma(k)} \in \mathcal{U}(\mathfrak{g}) \tag{14}$$

  from the symmetric algebra over $\mathfrak{g}$ into the universal enveloping algebra allows to pull the product of $\mathcal{U}(\mathfrak{g})$ back to $\mathrm{S}^\bullet(\mathfrak{g})$ and hence to polynomials on $\mathfrak{g}^*$. One can now show that after interpreting $\hbar$ as a formal parameter one indeed obtains a star product quantizing the linear Poisson bracket. This star product is completely characterized by the feature that

$$\exp(\hbar\xi) \star \exp(\hbar\eta) = \exp(\mathrm{BCH}(\hbar\xi, \hbar\eta)) \tag{15}$$

  for $\xi, \eta \in \mathfrak{g}$ with the Baker-Campbell-Hausdorff series BCH, see [19, 57].
- The next interesting example is perhaps the complex projective space $\mathbb{CP}^n$ and its non-compact dual, the Poincaré disc $\mathbb{D}_n$ with their canonical Kähler structures of constant holomorphic sectional curvature. For these, star products were considered by Moreno and Ortega-Navarro [72] who gave recursive formulas using local coordinates. Cahen, Gutt, and Rawnsley [30–33] discussed this in their series of papers of quantization of Kähler manifolds as one of the examples. The first explicit (non-recursive) formula was found in [17, 18] by a quantization of phase space reduction and extended to complex Grassmannians in [83]. Ever since these star products have been re-discovered by various authors.

We briefly comment on the general existence results: as already mentioned, the symplectic case was settled in the early 1980s. The Poisson case follows from Kontsevich's formality theorem.

Theorem 2.2 (Kontsevich) *On every Poisson manifold there exist star products.*

The classification is slightly more difficult to describe: we consider *formal Poisson structures*

$$\pi = \hbar\pi_1 + \hbar^2\pi_2 + \cdots \in \hbar\Gamma^\infty(\Lambda^2 TM)[[\hbar]] \quad \text{with} \quad [\![\pi, \pi]\!] = 0. \tag{16}$$

Moreover, let $X = \hbar X_1 + \hbar^2 X_2 + \cdots \in \hbar\Gamma^\infty(TM)[[\hbar]]$ be a formal vector field, starting in first order of $\hbar$. Then one calls $\exp(\mathscr{L}_X)$ a formal diffeomorphism which defines an action

$$\exp(\mathscr{L}_X)\colon \Gamma^\infty(\Lambda^2 TM)[[\hbar]] \ni \nu \;\mapsto\; \nu + \mathscr{L}_X\nu + \frac{1}{2}\mathscr{L}_X^2\nu + \cdots \in \Gamma^\infty(\Lambda^2 TM)[[\hbar]]. \tag{17}$$

Via the Baker-Campbell-Hausdorff series, the set of formal diffeomorphisms becomes a group and (17) is a group action. Since $\mathscr{L}_X$ is a derivation of the Schouten bracket, it follows that the action of $\exp(\mathscr{L}_X)$ preserves formal Poisson structures. The space of orbits of formal Poisson structures modulo this group action gives now the classification:

Theorem 2.3 (Kontsevich) *The set of equivalence classes of formal star products is in bijection to the set of equivalence classes of formal Poisson structures modulo formal diffeomorphisms.*

In general, both moduli spaces are extremely difficult to describe. However, if the first order term π_1 in π is symplectic, then we have a much easier description which is in fact entirely topological:

Theorem 2.4 (Bertelson, Cahen, Gutt, Nest, Tsygan, Deligne, ...) *On a symplectic manifold (M, ω) the equivalence classes of star products are in bijection to the formal series in the second deRham cohomology. In fact, one has a canonical surjective map*

$$c\colon \star \;\mapsto\; c(\star) \in \frac{[\omega]}{\mathrm{i}\hbar} + \mathrm{H}^2_{\mathrm{dR}}(M, \mathbb{C})[[\hbar]] \tag{18}$$

such that $\star$ and $\star'$ are equivalent iff $c(\star) = c(\star')$.

This map is now called the characteristic class of the symplectic star product. In a sense which can be made very precise [29], the inverse of $c(\star)$ corresponds to Kontsevich's classification by formal Poisson tensors.

3 Morita Classification

We come now to some more particular topics in deformation quantization. In this section we discuss a coarser classification result than the above classification up to equivalence.

The physical motivation to look for Morita theory is rather simple and obvious: in quantum theory we can not solely rely on the observable algebra as the only object of interest. Instead we also need to have a reasonable notion of states. While for C^*-algebras there is a simple definition of a state as a normalized positive functional, in deformation quantization we do not have C^*-algebras in a first step. Surprisingly, the notion of positive functionals still makes sense if interpreted in the sense of the ring-ordering of $\mathbb{R}[[\hbar]]$ and produces a physically reasonable definition of states, see [15]. However, the requirements from quantum theory do not stop here: we also need a super-position principle for states. Since positive functionals can only be added convexly, we need to realize the positive functionals as expectation value functionals for a *-representation of the observable algebra on some (pre-) Hilbert space. Then we can take complex linear combination of the corresponding vectors to implement the super-position principle. This leads to the need to understand the representation theory of the star product algebras, a program which was investigated in great detail [24, 25, 27–29, 60], see also [86] for a review. The main point is that replacing the ring of scalars from $\mathbb{R}$ to $\mathbb{R}[[\hbar]]$ and thus from $\mathbb{C}$ to $\mathbb{C}[[\hbar]]$ works surprisingly well as long as we do not try to implement analytic concepts: the non-archimedean order of $\mathbb{R}[[\hbar]]$ forbids a reasonable analysis. However, the concept of positivity is entirely algebraic and hence can be used and employed in this framework as well.

In fact, one does not need to stop here: *any* ordered ring R instead of $\mathbb{R}$ will do the job and one can study *-algebras over $\mathsf{C} = \mathsf{R}(\mathrm{i})$ and their *-representation theory on pre Hilbert modules over C. For many reasons it will also be advantageous to consider representation spaces where the inner product is not taking values in the scalars but in some *auxiliary* *-algebra $\mathcal{D}$.

Example Let $E \longrightarrow M$ be a complex vector bundle over a smooth manifold M. Then $\Gamma^\infty(E)$ is a $\mathscr{C}^\infty(M)$-module in the usual way. A Hermitian fiber metric h now gives a sesquilinear map

$$\langle \cdot, \cdot \rangle : \Gamma^\infty(E) \times \Gamma^\infty(E) \longrightarrow \mathscr{C}^\infty(M) \tag{19}$$

which is also $\mathscr{C}^\infty(M)$-linear in the second argument, i.e. we have $\langle s, tf \rangle = \langle s, t \rangle f$ for all $s, t \in \Gamma^\infty(E)$ and $f \in \mathscr{C}^\infty(M)$. Moreover, the pointwise positivity of h_p on E_p implies that the map

$$\langle \cdot, \cdot \rangle^{(n)} : \Gamma^\infty(E)^n \times \Gamma^\infty(E)^n \longrightarrow M_n(\mathscr{C}^\infty(M)) = \mathscr{C}^\infty(M, M_n(\mathbb{C})) \tag{20}$$

is positive for all n in the sense that the matrix-valued function $\langle S, S \rangle^{(n)} \in \mathscr{C}^\infty(M, M_n(\mathbb{C}))$ yields a positive matrix at all points of M for all $S = (s_1, \ldots, s_n) \in \Gamma^\infty(E)^n$.

Using this kind of *complete positivity* for an inner product yields the definition of a pre Hilbert right module over a *-algebra $\mathcal{D}$, where the inner product takes values in $\mathcal{D}$. Then again, we can formulate what are *-representations of a *-algebra $\mathcal{A}$ on such a pre Hilbert right module over $\mathcal{D}$. Without further difficulties this gives

various categories of *-representations of *-algebras on inner product modules or pre Hilbert modules over auxiliary *-algebras.

Having a good notion of *-representations of *-algebras it is a major talks to understand the resulting categories for those *-algebras occurring in deformation quantization. From C^*-algebra theory we anticipate that already with the full power of functional-analytic techniques it will in general be impossible to "understand" the category of *-representations completely, beside rather trivial examples. The reason is that there will simply be too many inequivalent such *-representations and a decomposition theory into irreducible ones is typically an extremely hard problem. In a purely algebraic situation like for formal star product algebras, things are even worse: here we expect even more inequivalent ones which are just artifacts of the algebraic formulation. There are many examples of inequivalent *-representations which, after one implements mild notions of convergence and hence of analytic aspects, become equivalent. From a physical point of view such inequivalences would then be negligible. However, it seems to be quite difficult to decide this *before* convergence is implemented, i.e. on the algebraic side.

Is the whole program now useless, hopeless? The surprising news is that one can indeed say something non-trivial about the *-representation theories of the star product algebras from deformation quantization, and for *-algebras in general. The idea is that even if the *-representation of a given *-algebra is horribly complicated and contains maybe unwanted *-representations, we can still *compare* the whole *-representation theory of one *-algebra to another *-algebra and ask whether they are equivalent as categories.

This is now the basic task of Morita theory. To get a first impression we neglect the additional structure of ordered rings, *-involutions, and positivity and consider just associative algebras over a common ring of scalars. For two such algebras $\mathcal{A}$ and $\mathcal{B}$ we want to know whether their categories of left modules are equivalent categories. Now there might be many very strange functors implementing an equivalence and hence one requires them to be compatible with direct sums of modules, which is clearly a reasonable assumption. The prototype of such a functor is then given by the tensor product with a $(\mathcal{B},\mathcal{A})$-bimodule. Since the tensor product with $\mathcal{A}$ itself is (for unital algebras) naturally isomorphic to the identity functor and since the tensor product of bimodules is associative up to a natural isomorphism, the question of equivalence of categories via such tensor product functors becomes equivalent to the question of *invertible bimodules*: Here a $(\mathcal{B},\mathcal{A})$-bimodule ${}_{\mathcal{B}}\mathcal{E}_{\mathcal{A}}$ is called invertible if there is an $(\mathcal{A},\mathcal{B})$-bimodule ${}_{\mathcal{A}}\mathcal{E}'_{\mathcal{B}}$ such that the tensor product ${}_{\mathcal{B}}\mathcal{E}_{\mathcal{A}} \otimes_{\mathcal{A}} {}_{\mathcal{A}}\mathcal{E}'_{\mathcal{B}}$ is isomorphic to $\mathcal{B}$ and ${}_{\mathcal{A}}\mathcal{E}'_{\mathcal{B}} \otimes_{\mathcal{B}} {}_{\mathcal{B}}\mathcal{E}_{\mathcal{A}}$ is isomorphic to $\mathcal{A}$, always as bimodules.

The classical theorem of Morita now gives a complete and fairly easy description of the possible bimodules with this property: ${}_{\mathcal{B}}\mathcal{E}_{\mathcal{A}}$ has to be a finitely generated projective and full right $\mathcal{A}$-module and $\mathcal{B}$ is isomorphic to $\mathsf{End}_{\mathcal{A}}({}_{\mathcal{A}}\mathcal{E})$ via the left module structure, see e.g. [69].

Now the question is how such bimodules look like for star product algebras. Classically, the finitely generated projective modules over $\mathscr{C}^\infty(M)$ are, up to isomorphism, just sections $\Gamma^\infty(E)$ of a vector bundle $E \longrightarrow M$. This is the

famous Serre-Swan theorem in its incarnation for differential geometry. As soon as the fiber dimension is non-zero, the fullness condition is trivially satisfied. Hence the only Morita equivalent algebras to $\mathscr{C}^\infty(M)$ are, again up to isomorphism, the sections $\Gamma^\infty(\mathsf{End}(E))$ of endomorphism bundles. The corresponding bimodule is then $\Gamma^\infty(E)$ on which both algebras act in the usual way. It now requires a little argument to see that for star products, an equivalence bimodule gives an equivalence bimodule in the classical limit $\hbar = 0$, i.e. a vector bundle. Conversely, the sections of every vector bundle can be deformed into a right module over the star product algebra in a unique way up to isomorphism. Thus for star products, we have to look for the corresponding module endomorphisms of such deformed sections of vector bundles. Finally, in order to get again a star product algebra, the endomorphisms of the deformed sections have to be, in the classical limit, isomorphic to the functions on a manifold again. This can only happen if the vector bundle was actually a line bundle over the same manifold. Hence the remaining task is to actually compute the star product of the algebra acting from the left side when the star product for the algebra on the right side is known. Here one has the following results:

Theorem 3.1 (Bursztyn, W. [26]) *Let (M, ω) and (M', ω') be a symplectic manifolds and let $\star$, $\star'$ be two star products on M and M', respectively. Then $\star$ and $\star'$ are Morita equivalent iff there exists a symplectomorphism $\psi : M \longrightarrow M'$*

$$\psi^* c(\star') - c(\star) \in 2\pi \mathrm{i} \mathrm{H}^2_{\mathrm{dR}}(M, \mathbb{Z}). \tag{21}$$

The difference of the above classes defines then a line bundle which implements the Morita equivalence bimodule by deforming its sections.

This theorem already has an important physical interpretation: for cotangent bundles T^*Q the characteristic classes $c(\star)$ can be interpreted as the classes of magnetic fields B on the configuration space Q. Then a quantization of a charged particle in the background field of such a B requires a star product with characteristic class $c(\star)$. Compared to the trivial characteristic class, $c(\star) = 0$, the above theorem then tells that quantization with magnetic field has the same representation theory iff the magnetic field satisfies the integrality condition for a Dirac monopole. Thus we get a Morita theoretic interpretation of the charge quantization for magnetic monopoles which is now extremely robust against details of the quantization procedure: the statement holds for all cotangent bundles and for all equivalent star products with the given characteristic class.

Also in the more general Poisson case the full classification is known. Here the actual statement is slightly more technical as it requires the Kontsevich class of the star products and a canonically given action of the deRham cohomology on equivalence classes of formal Poisson structures by gauge transformations. Then one obtains the following statement:

Theorem 3.2 (Bursztyn, Dolgushev, W. [29]) *Star products on Poisson manifolds are Morita equivalent iff their Kontsevich classes of formal Poisson tensors are gauge equivalent by a $2\pi\mathrm{i}$-integral deRham class.*

4 Beyond Formal Star Products

Since formal star products are clearly not sufficient for physical purposes, one has to go beyond formal power series. Here several options are available: on one hand one can replace the formal series in the star products by integral formulas. The formal series can then be seen as the asymptotic expansions of the integral formulas in the sense of Taylor series of smooth functions of $\hbar$, which are typically not analytic: hence we cannot expect convergence. Nevertheless, the integral formulas allow for a good analytic framework.

However, if one moves to field theories and hence to infinite-dimensional systems, quantization becomes much more complicated. Surprisingly, series formulas for star products can still make sense in certain examples, quite unlike the integral formulas: such integrals would consist of integrations over a infinite-dimensional phase space. Hence we know that such things can hardly exist in a mathematically sound way.

This motivates the second alternative, namely to investigate the formal series in the star products directly without integral formulas in the back. This might also be possible in infinite dimensions and yield reasonable quantizations there. While this is a program far from being understood, we now present a class of examples with a particular physical relevance: the Weyl algebra.

Here we consider a real vector space V with a bilinear map $\Lambda\colon V \times V \longrightarrow \mathbb{C}$. Then we consider the complexified symmetric algebra $\mathrm{S}^\bullet_{\mathbb{C}}(V)$ of V and interpret this as the polynomials on the dual V^*. In finite dimensions this is correct, in infinite dimensions the symmetric algebra is better to be interpreted as the polynomials on the (not necessarily existing) pre-dual. On V^*, there are simply much more polynomials than the ones arising from $\mathrm{S}^\bullet_{\mathbb{C}}(V)$. Now we can extend Λ to a biderivation

$$P_\Lambda\colon \mathrm{S}^\bullet_{\mathbb{C}}(V) \otimes \mathrm{S}^\bullet_{\mathbb{C}}(V) \longrightarrow \mathrm{S}^\bullet_{\mathbb{C}}(V) \otimes \mathrm{S}^\bullet_{\mathbb{C}}(V) \tag{22}$$

in a unique way by enforcing the Leibniz rule in both tensor factors. If we denote by $\mu\colon \mathrm{S}^\bullet_{\mathbb{C}}(V) \otimes \mathrm{S}^\bullet_{\mathbb{C}}(V) \longrightarrow \mathrm{S}^\bullet_{\mathbb{C}}(V)$ the symmetric tensor product, then

$$\{a, b\}_\Lambda = \mu \circ (P_\Lambda(a \otimes b) - P_\Lambda(b \otimes a)) \tag{23}$$

is a Poisson bracket. In fact, this is the unique constant Poisson bracket with the property that for linear elements $v, w \in V$ we have $\{v, w\} = \Lambda(v, w) - \Lambda(w, v)$. Hence the antisymmetric part of Λ determines the bracket. However, we will use the symmetric part for defining the star product. This will allow to include also standard-orderings or other orderings like Wick ordering from the beginning.

A star product quantizing this constant Poisson structure can then be found easily. We set

$$a \star b = \mu \circ \exp(zP_\Lambda)(a \otimes b) \tag{24}$$

where $z \in \mathbb{C}$ is the deformation parameter. For physical applications we will have to set $z = \frac{i\hbar}{2}$ later on. Note that $\star$ is indeed well-defined since on elements in the symmetric algebra, the operator P_Λ lowers the degree by one in each tensor factor.

In a next step we want to extend this product to more interesting functions than the polynomial-like ones. The strategy is to look for a topology which makes the product continuous and which allows for a large completion of $\mathrm{S}^\bullet_{\mathbb{C}}(V)$. To start with, one has to assume that V is endowed with a topology itself. Hence let V be a locally convex Hausdorff space. In typical examples from quantum mechanics, V is the (dual of the) phase space and hence finite dimensional, which makes the topology unique. In quantum field theory, V would be something like test function spaces, i.e. either the Schwartz space $\mathcal{S}(\mathbb{R}^d)$ or $\mathscr{C}^\infty_0(M)$ for a manifold M, etc. In this case V would be a Fréchet or LF space.

We use now the continuous seminorms of V to extend them to tensor powers $V^{\otimes k}$ for all $k \in \mathbb{N}$ by taking their tensor powers: we equip $V^{\otimes k}$ with the π-topology inherited from V. This means that for a continuous seminorm p on V we consider $p^{\otimes k}$ on $V^{\otimes k}$ and take all such seminorms to define a locally convex topology on $V^{\otimes k}$. Viewing the symmetric tensor powers as a subspace, this induces the π-topology also for $\mathrm{S}^\bullet_{\mathbb{C}}(V)$, simply by restricting the seminorms $p^{\otimes k}$. For the whole symmetric algebra we need to extend the seminorms we have on each symmetric degree. This can be done in many inequivalent ways. Useful for our purposes is the following construction. We fix a parameter $R \geq \frac{1}{2}$ and define

$$p_R(a) = \sum_{k=0}^{\infty} k!^R p^{\otimes k}(a_k) \tag{25}$$

for every $a = \sum_{k=0}^{\infty} a_k$ with $a_k \in \mathrm{S}^k_{\mathbb{C}}(V)$. Note that the sum is finite as long as we take a in the symmetric algebra. Now taking all those seminorms p_R for all continuous seminorms p of V induces a locally convex topology on V. Clearly, this is again Hausdorff. Moreover, all $\mathrm{S}^k_{\mathbb{C}}(V)$ are closed embedded subspaces in $\mathrm{S}^\bullet_{\mathbb{C}}(V)$ with respect to this topology.

The remarkable property of this topology is now that a continuous Λ will induce a continuous star product [88]:

Theorem 4.1 *Let $\Lambda\colon V \times V \longrightarrow \mathbb{C}$ be a continuous bilinear form on V. Then $\star$ is a continuous associative product on $\mathrm{S}^\bullet_{\mathbb{C}}(V)$ with respect to the locally convex topology induced by all the seminorms p_R with p being a continuous seminorm on V, as long as $R \geq \frac{1}{2}$.*

The proof consists in an explicit estimate for $a \star b$. Note that the topology can *not* be locally multiplicatively convex since in the Weyl algebra we have elements satisfying canonical commutation relations, thereby forbidding a submultiplicative seminorm.

Definition 4.2 (Locally convex Weyl algebra) Let $\Lambda\colon V \times V \longrightarrow \mathbb{C}$ be a continuous bilinear form on V. Then the completion of $\mathrm{S}^\bullet_{\mathbb{C}}(V)$ with respect to the above

locally convex topology and with the canonical extension of $\star$ is called the locally convex Weyl algebra $\mathcal{W}_R(V, \star)$.

Thus we have found a framework where the Weyl star product actually converges. Without proofs we list a few properties of this Weyl algebra:

- The locally convex Weyl algebra $\mathcal{W}_R(V, \star)$ is a locally convex unital associative algebra. The product $a \star b$ can be written as the absolutely convergent series

$$a \star b = \mu \circ \exp(zP_\Lambda)(a \otimes b). \tag{26}$$

- The product $\star$ depends holomorphically on $z \in \mathbb{C}$.
- For $\frac{1}{2} \leq R < 1$ the locally convex Weyl algebra $\mathcal{W}_R(V, \star)$ contains the exponential functions $\mathrm{e}^{\alpha v}$ for all $v \in V$ and all $\alpha \in \mathbb{C}$. They satisfy the usual Weyl relations. Note that not only the unitary ones, i.e. for α imaginary, are contained in the Weyl algebra, but all exponentials.
- The locally convex Weyl algebra is nuclear iff V is nuclear. In all relevant examples in quantum theory this will be the case. In this case we refer to the *nuclear Weyl algebra*.
- If V admits an absolute Schauder basis, then the symmetrized tensor products of the basis vectors constitute an absolute Schauder basis for the Weyl algebra, too. Again, in many situations V has such a basis.
- The Weyl algebras for different Λ on V are isomorphic if the antisymmetric parts of the bilinear forms coincide.
- Evaluations at points in the topological dual V' are continuous linear functionals on $\mathcal{W}_R(V, \star)$. Hence we still can view the elements of the completion as particular functions on V'.
- The translations by elements in V' still act on $\mathcal{W}_R(V, \star)$ by continuous automorphisms. If $R < 1$ these translations are inner automorphism as soon as the element $\varphi \in V'$ is in the image of the musical map induced by Λ.

We now conclude this section with a few comments on examples. First it is clear that in finite dimensions we can take $V = \mathbb{R}^{2n}$ with the canonical Poisson bracket on the symmetric algebra. Then many types of orderings can be incorporated in fixing the symmetric part of Λ, while the antisymmetric part is given by the Poisson bracket. Thus all the resulting star products allow for this analytic framework. This includes examples known earlier in the literature, see e.g. [6, 80]. In this case we get a nuclear Weyl algebra with an absolute Schauder basis.

More interesting is of course the infinite dimensional case. Here we have to specify the space V and the bilinear form Λ more carefully. In fact, the *continuity* of Λ becomes now a strong conditions since bilinear maps in locally convex analysis tend to be only separately continuous without being continuous. However, there are several situations where we can either conclude the continuity of a bilinear separately continuous map by abstract arguments, like for Fréchet spaces. Or one can show directly that the particular bilinear form one is interested in is continuous. We give one of the most relevant examples for (quantum) field theory:

Example Let M be a globally hyperbolic spacetime and let D be a normally hyperbolic differential operator acting on a real vector bundle E with fiber metric h. Moreover, we assume that D is a connection Laplacian for a metric connection with respect to h plus some symmetric operator B of order zero. In all relevant examples this is easy to obtain. Then one has advanced and retarded Green operators leading to the propagator F_M acting on test sections $\Gamma_0^\infty(E^*)$. We take $V = \Gamma_0^\infty(E^*)$ with its usual LF topology. Then

$$\Lambda(\varphi, \psi) = \int_M h^{-1}(F_M(\varphi), \psi)\mu_g \tag{27}$$

is the bilinear form leading to the Peierls bracket on the symmetric algebra $\mathrm{S}^\bullet(V)$. Here μ_g is the metric density as usual. The kernel theorem then guarantees that Λ is continuous as needed. Thus we obtain a locally convex and in fact nuclear Weyl algebra from this. Now Λ is highly degenerated. It follows that in the Poisson algebra there are many Casimir elements. The kernel of F_M generates a Poisson ideal and also an ideal in the Weyl algebra, which coincides with the vanishing ideal of the solution space. Hence dividing by this (Poisson) ideal gives a Poisson algebra or Weyl algebra which can be interpreted as the observables of the (quantum) field theory determined by the wave equation $Du = 0$. It can then be shown that for every Cauchy surface Σ in M there is a canonical algebra isomorphism to the Weyl algebra build from the symplectic Poisson algebra on the initial conditions on Σ. Details of this construction can be found in [88], see also [4] for the background information on the wave equation.

Acknowledgements It is a pleasure to thank the organizers of the Regensburg conference for their kind invitation and the fantastic organization of this stimulating conference. Moreover, I would like to thank Chiara Esposito and the Referee for helpful remarks on the manuscript.

References

1. A. Alekseev, E. Meinrenken, On the Kashiwara-Vergne conjecture. Invent. Math. **164**(3), 615–634 (2006). MR 2221133
2. A. Alekseev, C. Torossian, Kontsevich deformation quantization and flat connections. Commun. Math. Phys. **300**, 47–64 (2010). MR 2725182
3. A. Alekseev, C. Torossian, The Kashiwara-Vergne conjecture and Drinfeld's associators. Ann. Math. **175**(2), 415–463 (2012). MR 2877064
4. C. Bär, N. Ginoux, F. Pfäffle, *Wave Equations on Lorentzian Manifolds and Quantization*. ESI Lectures in Mathematics and Physics (European Mathematical Society (EMS), Zürich, 2007). MR MR2298021
5. F. Bayen, M. Flato, C. Frønsdal, A. Lichnerowicz, D. Sternheimer, Deformation theory and quantization. Ann. Phys. **111**, 61–151 (1978)
6. S. Beiser, H. Römer, S. Waldmann, Convergence of the Wick star product. Commun. Math. Phys. **272**, 25–52 (2007)
7. F.A. Berezin, General concept of quantization. Commun. Math. Phys. **40**, 153–174 (1975)
8. F.A. Berezin, Quantization. Math. USSR Izvestija **8**(5), 1109–1165 (1975)

9. F.A. Berezin, Quantization in complex symmetric spaces. Math. USSR Izvestija **9**(2), 341–379 (1975)
10. M. Bertelson, M. Cahen, S. Gutt, Equivalence of star products. Class. Quantum Gravity **14**, A93–A107 (1997)
11. P. Bieliavsky, Strict quantization of solvable symmetric spaces. J. Symplectic Geom. **1**(2), 269–320 (2002). MR MR1959584
12. P. Bieliavsky, S. Detournay, Ph. Spindel, The deformation quantizations of the hyperbolic plane. Commun. Math. Phys. **289**(2), 529–559 (2009). MR MR2506761
13. P. Bieliavsky, M. Massar, Oscillatory integral formulae for left-invariant star products on a class of Lie groups. Lett. Math. Phys. **58**, 115–128 (2001)
14. M. Bordemann, S. Waldmann, A fedosov star product of wick type for Kähler manifolds. Lett. Math. Phys. **41**, 243–253 (1997). MR MR1463874
15. M. Bordemann, S. Waldmann, Formal GNS construction and states in deformation quantization. Commun. Math. Phys. **195**, 549–583 (1998). MR MR1641003
16. M. Bordemann, E. Meinrenken, M. Schlichenmaier, Toeplitz quantization of Kähler manifolds and $gl(N), N \to \infty$ limit. Commun. Math. Phys. **165**, 281–296 (1994)
17. M. Bordemann, M. Brischle, C. Emmrich, S. Waldmann, Phase space reduction for star products: an explicit construction for $\mathbb{C}P^n$. Lett. Math. Phys. **36**, 357–371 (1996). MR MR1384642
18. M. Bordemann, M. Brischle, C. Emmrich, S. Waldmann, Subalgebras with converging star products in deformation quantization: an algebraic construction for $\mathbb{C}P^n$. J. Math. Phys. **37**, 6311–6323 (1996). MR MR1419171
19. M. Bordemann, N. Neumaier, S. Waldmann, Homogeneous fedosov star products on cotangent bundles I: Weyl and standard ordering with differential operator representation. Commun. Math. Phys. **198**, 363–396 (1998). MR MR1668901
20. M. Bordemann, N. Neumaier, S. Waldmann, Homogeneous fedosov star products on cotangent bundles II: GNS representations, the WKB expansion, traces, and applications. J. Geom. Phys. **29**, 199–234 (1999). MR MR1670009
21. M. Bordemann, N. Neumaier, M.J. Pflaum, S. Waldmann, On representations of star product algebras over cotangent spaces on hermitian line bundles. J. Funct. Anal. **199**, 1–47 (2003). MR MR1966822
22. R. Brunetti, K. Fredenhagen, R. Verch, The generally covariant locality principle—a new paradigm for local quantum field theory. Commun. Math. Phys. **237**, 31–68 (2003). MR MR2007173
23. R. Brunetti, K. Fredenhagen, P.L. Ribeiro, Algebraic structure of classical field theory I: kinematics and linearized dynamics for real scalar fields. **arXiv:1209.2148** (2012, preprint), 53
24. H. Bursztyn, S. Waldmann, *-ideals and formal Morita equivalence of *-algebras. Int. J. Math. **12**(5), 555–577 (2001). MR MR1843866
25. H. Bursztyn, S. Waldmann, Algebraic Rieffel induction, formal Morita equivalence and applications to deformation quantization. J. Geom. Phys. **37**, 307–364 (2001). MR MR1811148
26. H. Bursztyn, S. Waldmann, The characteristic classes of Morita equivalent star products on symplectic manifolds. Commun. Math. Phys. **228**, 103–121 (2002). MR MR1911250
27. H. Bursztyn, S. Waldmann, Bimodule deformations, Picard groups and contravariant connections. K-Theory **31**, 1–37 (2004). MR MR2050877
28. H. Bursztyn, S. Waldmann, Completely positive inner products and strong Morita equivalence. Pac. J. Math. **222**, 201–236 (2005). MR MR2225070
29. H. Burzstyn, V. Dolgushev, S. Waldmann, Morita equivalence and characteristic classes of star products. Crelle's J. Reine Angew. Math. **662**, 95–163 (2012)
30. M. Cahen, S. Gutt, J. Rawnsley, Quantization of Kähler manifolds I: geometric interpretation of Berezin's quantization. J. Geom. Phys. **7**, 45–62 (1990)
31. M. Cahen, S. Gutt, J. Rawnsley, Quantization of Kähler manifolds. II. Trans. Am. Math. Soc. **337**(1), 73–98 (1993)

32. M. Cahen, S. Gutt, J. Rawnsley, Quantization of Kähler manifolds. III. Lett. Math. Phys. **30**, 291–305 (1994)
33. M. Cahen, S. Gutt, J. Rawnsley, Quantization of Kähler manifolds. IV. Lett. Math. Phys. **34**, 159–168 (1995)
34. A. Cannas da Silva, A. Weinstein, *Geometric Models for Noncommutative Algebras*. Berkeley Mathematics Lecture Notes (AMS, Providence, 1999)
35. A.S. Cattaneo, Formality and star products, in *Poisson Geometry, Deformation Quantisation and Group Representations*, ed. by S. Gutt, J. Rawnsley, D. Sternheimer. London Mathematical Society Lecture Note Series, vol. 323 (Cambridge University Press, Cambridge, 2005), pp. 79–144. Lecture Notes taken by D. Indelicato
36. A.S. Cattaneo, G. Felder, L. Tomassini, From local to global deformation quantization of Poisson manifolds. Duke Math. J. **115**(2), 329–352 (2002)
37. P. Deligne, Déformations de l'algèbre des fonctions d'une variété symplectique: comparaison entre fedosov et dewilde, lecomte. Sel. Math. New Ser. **1**(4), 667–697 (1995)
38. M. DeWilde, P.B.A. Lecomte, Star-produits et déformations formelles associées aux variétés symplectiques exactes. C. R. Acad. Sc. Paris **296**, 825–828 (1983)
39. M. DeWilde, P.B.A. Lecomte, Existence of star-products and of formal deformations of the poisson lie algebra of arbitrary symplectic manifolds. Lett. Math. Phys. **7**, 487–496 (1983)
40. M. DeWilde, P.B.A. Lecomte, Star-products on cotangent bundles. Lett. Math. Phys. **7**, 235–241 (1983)
41. J. Dito, Star-product approach to quantum field theory: the free scalar field. Lett. Math. Phys. **20**, 125–134 (1990)
42. J. Dito, Star-products and nonstandard quantization for Klein-Gordon equation. J. Math. Phys. **33**(2), 791–801 (1992)
43. J. Dito, An example of cancellation of infinities in the star-quantization of fields. Lett. Math. Phys. **27**, 73–80 (1993)
44. V.A. Dolgushev, Covariant and equivariant formality theorems. Adv. Math. **191**, 147–177 (2005). MR MR2102846
45. V.A. Dolgushev, V.N. Rubtsov, An algebraic index theorem for Poisson manifolds. J. Reine Angew. Math. **633**, 77–113 (2009). MR 2561197
46. V. Dolgushev, D. Tamarkin, B. Tsygan, The homotopy Gerstenhaber algebra of Hochschild cochains of a regular algebra is formal. J. Noncommut. Geom. **1**(1), 1–25 (2007). MR MR2294189
47. V.G. Drinfel'd, On constant quasiclassical solutions of the Yang-Baxter quantum equation. Sov. Math. Dokl. **28**, 667–671 (1983)
48. J.-P. Dufour, N.T. Zung, *Poisson Structures and Their Normal Forms*. Progress in Mathematics, vol. 242 (Birkhäuser Verlag, Basel/Boston/New York, 2005). MR MR2178041
49. M. Dütsch, K. Fredenhagen, A local (perturbative) construction of observables in gauge theories: the example of QED. Commun. Math. Phys. **203**, 71–105 (1999)
50. M. Dütsch, K. Fredenhagen, Algebraic quantum field theory, perturbation theory, and the loop expansion. Commun. Math. Phys. **219**, 5–30 (2001)
51. M. Dütsch, K. Fredenhagen, Perturbative algebraic field theory, and deformation quantization. Field Inst. Commun. **30**, 151–160 (2001)
52. C. Esposito, *Formality Theory. From Poisson Structures to Deformation Quantization* (Springer, Heidelberg/Berlin, 2015)
53. B.V. Fedosov, Quantization and the index. Sov. Phys. Dokl. **31**(11), 877–878 (1986)
54. B.V. Fedosov, A simple geometrical construction of deformation quantization. J. Diff. Geom. **40**, 213–238 (1994)
55. B.V. Fedosov, *Deformation Quantization and Index Theory* (Akademie Verlag, Berlin, 1996)
56. H.J. Groenewold, On the principles of elementary quantum mechanics. Physica **12**, 405–460 (1946)
57. S. Gutt, An explicit $*$-product on the cotangent bundle of a lie group. Lett. Math. Phys. **7**, 249–258 (1983)

58. S. Gutt, J. Rawnsley, Equivalence of star products on a symplectic manifold; an introduction to deligne's čech cohomology classes. J. Geom. Phys. **29**, 347–392 (1999)
59. S. Hollands, R.M. Wald, Axiomatic quantum field theory in curved spacetime. Commun. Math. Phys. **293**(1), 85–125 (2010). MR 2563799
60. S. Jansen, S. Waldmann, The H-covariant strong Picard groupoid. J. Pure Appl. Algebra **205**, 542–598 (2006). MR MR2210219
61. A.V. Karabegov, Deformation quantization with separation of variables on a Kähler manifold. Commun. Math. Phys. **180**, 745–755 (1996)
62. A.V. Karabegov, On Fedosov's approach to deformation quantization with separation of variables, in *Conférence Moshé Flato 1999. Quantization, Deformations, and Symmetries*, ed. by G. Dito and D. Sternheimer. Mathematical Physics Studies, vol. 22 (Kluwer Academic, Dordrecht/Boston/London, 2000)
63. M. Kontsevich, Deformation quantization of poisson manifolds, I. **q-alg/9709040** (1997, preprint)
64. M. Kontsevich, Formality conjecture, in *Deformation Theory and Symplectic Geometry*, ed. by D. Sternheimer, J. Rawnsley, S. Gutt. Mathematical Physics Studies, vol. 20 (Kluwer Academic, Dordrecht/Boston/London, 1997), pp. 139–156
65. M. Kontsevich, Operads and motives in deformation quantization. Lett. Math. Phys. **48**, 35–72 (1999)
66. M. Kontsevich, Deformation quantization of algebraic varieties. Lett. Math. Phys. **56**, 271–294 (2001)
67. M. Kontsevich, Deformation quantization of Poisson manifolds. Lett. Math. Phys. **66**, 157–216 (2003)
68. M. Kontsevich, Y. Soibelman, Deformations of algebras over operads and the Deligne conjecture, in *Conférence Moshé Flato 1999. Quantization, Deformations, and Symmetries*, ed. by G. Dito, D. Sternheimer. Mathematical Physics Studies, vol. 21 (Kluwer Academic, Dordrecht/Boston/London, 2000), pp. 255–307
69. T.Y. Lam, *Lectures on Modules and Rings*. Graduate Texts in Mathematics, vol. 189 (Springer, Berlin/Heidelberg/New York, 1999)
70. N.P. Landsman, *Mathematical Topics Between Classical and Quantum Mechanics*. Springer Monographs in Mathematics (Springer, Berlin/Heidelberg/New York, 1998)
71. C. Laurent-Gengoux, A. Pichereau, P. Vanhaecke, *Poisson Structures*. Grundlehren der mathematischen Wissenschaften, vol. 347 (Springer, Heidelberg/Berlin/New York, 2013)
72. C. Moreno, P. Ortega-Navarro, $*$-products on $d^1()$, s^2 and related spectral analysis. Lett. Math. Phys. **7**, 181–193 (1983)
73. J.E. Moyal, Quantum mechanics as a statistical theory. Proc. Camb. Philos. Soc. **45**, 99–124 (1949)
74. T. Natsume, *C^*-algebraic deformation quantization of closed Riemann surfaces*, C^*-algebras, ed. by J. Cuntz, S. Echterhoff (Springer, Berlin, 2000). Proceedings of the SFB Workshop held at the University of Münster, Münster, 8–12 March 1999, pp. 142–150, MR MR1796906
75. T. Natsume, R. Nest, Topological approach to quantum surfaces. Commun. Math. Phys. **202**, 65–87 (1999)
76. T. Natsume, R. Nest, I. Peter, Strict quantizations of symplectic manifolds. Lett. Math. Phys. **66**, 73–89 (2003)
77. R. Nest, B. Tsygan, Algebraic index theorem. Commun. Math. Phys. **172**, 223–262 (1995)
78. N. Neumaier, Local ν-Euler derivations and Deligne's characteristic class of Fedosov star products and star products of special type. Commun. Math. Phys. **230**, 271–288 (2002)
79. N. Neumaier, Universality of fedosov's construction for star products of wick type on pseudo-Kähler manifolds. Rep. Math. Phys. **52**, 43–80 (2003)
80. H. Omori, Y. Maeda, N. Miyazaki, A. Yoshioka, Orderings and non-formal deformation quantization. Lett. Math. Phys. **82**, 153–175 (2007). MR MR2358466
81. M.A. Rieffel, Deformation quantization of Heisenberg manifolds. Commun. Math. Phys. **122**, 531–562 (1989)

82. M.A. Rieffel, Deformation quantization for actions of $\mathbb{R}^d$. Mem. Am. Math. Soc. **106**(506), 93pp (1993). MR MR1184061
83. J. Schirmer, *A Star Product for Complex Grassmann Manifolds*, Freiburg FR-THEP-97/21 **q-alg/9709021** (1997, preprint)
84. D. Tamarkin, *Another Proof of M. Kontsevich Formality Theorem*, **arXiv:math/9803025** (1998, preprint), 24
85. I. Vaisman, *Lectures on the Geometry of Poisson Manifolds* (Birkhäuser Verlag, Basel/Boston/Berlin, 1994)
86. S. Waldmann, States and representation theory in deformation quantization. Rev. Math. Phys. **17**, 15–75 (2005). MR MR2130623
87. S. Waldmann, *Poisson-Geometrie und Deformationsquantisierung. Eine Einführung* (Springer, Heidelberg/Berlin/New York, 2007)
88. S. Waldmann, A nuclear Weyl algebra. J. Geom. Phys. **81**, 10–46 (2014). MR MR3194213
89. H. Weyl, *The Theory of Groups and Quantum Mechanics* (Dover, New York, 1931)

Dirac's Point Electron in the Zero-Gravity Kerr–Newman World

Michael K.-H. Kiessling and A. Shadi Tahvildar-Zadeh

Contents

Abstract The results of a study of the Dirac Hamiltonian for a point electron in the zero-gravity Kerr–Newman spacetime are reported; here, "zero-gravity" means $G \to 0$, where G is Newton's constant of universal gravitation, and the limit is effected in the Boyer–Lindquist coordinate chart of the maximal analytically extended, topologically nontrivial, Kerr–Newman spacetime. In a nutshell, the results are: the essential self-adjointness of the Dirac Hamiltonian; the reflection symmetry about zero of its spectrum; the location of the essential spectrum, exhibiting a gap about zero; and (under two smallness assumptions on some parameters) the existence of a point spectrum in this gap, corresponding to bound

This is an expanded version of the talk titled "The Dirac equation and the Kerr-Newman spacetime," given by the first author at the Quantum Mathematical Physics conference.

M.K.-H. Kiessling (✉) • A.S. Tahvildar-Zadeh
Department of Mathematics, Rutgers, The State University of New Jersey, Piscataway, NJ, USA
e-mail: miki@math.rutgers.edu; shadi@math.rutgers.edu

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_19

states of Dirac's point electron in the electromagnetic field of the zero-G Kerr–Newman ring singularity. The symmetry result of the spectrum extends to the Dirac Hamiltonian for a point electron in a generalization of the zero-G Kerr–Newman spacetime with different ratio of electric-monopole to magnetic-dipole moment. The results are discussed in the context of the general-relativistic hydrogen problem. Also, some interesting projects for further inquiry are listed in the last section.

Keywords Kerr–Newman spacetime • Dirac electron • Zero-gravity limit

Mathematics Subject Classification (2010). 81, 83, 35.

1 Introduction

There are many studies of Dirac's wave equation on curved background spacetimes, see e.g. [4–7, 10, 12, 14–16, 20–23, 36, 37, 39, 42, 51–53]. The papers [2–4, 6, 7, 20–23, 39, 45, 51, 52] in particular deal with Dirac's equation on some member of the Kerr–Newman family of spacetimes. However, to the best of our knowledge, nobody has yet investigated Dirac's equation on the entire maximal analytically extended, topologically nontrivial Kerr–Newman spacetime. Such an investigation faces many conceptual and technical obstacles, but it becomes feasible in a zero-gravity limit which preserves the nontrivial topology of the Kerr–Newman spacetime and its associated electromagnetic structures. In this limit one can rigorously study these general-relativistic effects on the Dirac Hamiltonian, separated from—and not obscured by—those caused by general-relativistic gravity. The results of such a zero-gravity investigation [32, 47] are reported here.

Readers whose expertise includes hyperbolic partial differential equations on nontrivial background spacetimes, and who right away want to find out about the results that we have obtained, may now want to jump to the technical Sect. 3. Readers with expertise elsewhere in mathematical physics may find the few introductory lines written above hardly motivating enough to read on, however. Fortunately, a study of Dirac's equation on a zero-gravity Kerr–Newman spacetime can be motivated in at least two different other ways, one of which we are going to elaborate on in the next section. There we discuss the *perplexing problem* of the general-relativistic hydrogen spectrum, which ought to be interesting to most mathematical quantum physicists.[1] Yet another way to motivate our study—which is even more intriguing, but was not yet ready for public announcement

[1] We are not suggesting that experimental physicists should not worry about this academic problem. For the empirically relevant problem to estimate the influence of, say, Earth's gravitational field on the spectrum of hydrogen in the lab, see Papapetrou [40].

at the time of the Regensburg conference and is, therefore, only briefly mentioned here (in the last section)—has meanwhile been made public in our paper [31].

Our results are stated informally in the context of the general-relativistic hydrogen problem at the end of the next section, while the precise statements and some technical details are given in Sect. 3. In Sect. 4 we list open questions left unanswered by our study, and we indicate the key idea of [31].

2 On the General-Relativistic Hydrogen Spectrum

Hydrogen has played a crucial role in the development of the quantum theory of atomic spectra, and presumably this simplest of the chemical atoms will continue to play an important role in the ongoing efforts to find a more satisfactory theory; for instance, one that does not rely on artificial UV cutoffs, etc. Yet we do not have to venture into the realm of quantum field theory or quantum gravity to encounter perplexing issues that await clarification. We simply ask for a general-relativistic counterpart of the special-relativistic spectrum of the quantum mechanical Dirac Hamiltonian for an electron (modeled as a point charge) in the electromagnetic field of a proton (modeled either as a point—or spherical—charge, or as a combination of electric charge plus current distribution to account also for the proton's magnetic dipole field). Since gravity is very weak one would expect the general-relativistic Dirac point spectrum to differ from Sommerfeld's fine structure formula only by the tiniest amounts, and in particular to be computable perturbatively using Newton's constant of universal gravitation, G, as expansion parameter. But if that is indeed what one expects, then one will be in for a surprise!

2.1 The Coulomb Approximation

In this subsection only the electric field of the proton is considered. To have a reference point, we begin by recalling the spectral results of the familiar textbook problem, which is Dirac's equation for a point electron in flat Minkowski spacetime equipped with a proton, modeled as a point charge having a straight worldline; in the rest frame of this model proton the electron experiences only the electrostatic Coulomb field of the point charge. Subsequently we turn to the general-relativistic version of this problem.

The Special-Relativistic Spectrum

The pertinent Dirac Hamiltonian with domain[2] $C_c^\infty(\mathbb{R}^3\backslash\{\mathbf{0}\})^4$ is essentially self-adjoint on $L^2(\mathbb{R}^3\backslash\{\mathbf{0}\})^4$ with spectrum $\sigma = \sigma_{\rm ac} \cup \sigma_{\rm pp}$, the absolutely continuous part of which is given by

$$\sigma_{\rm ac} = (-\infty, -m] \cup [m, \infty), \tag{1}$$

where m is the empirical mass of the electron, while the discrete (here equal to the pure point) part is given by Sommerfeld's famous fine structure formula

$$\begin{aligned}\sigma_{\rm pp} &= \left\{ mc^2 \left(1 + \frac{\alpha_{\rm s}^2}{\left(n - \kappa + \sqrt{\kappa^2 - \alpha_{\rm s}^2}\right)^2} \right)^{-1/2} \right\}_{\substack{n=1,\dots,\infty \\ \kappa=1,\dots,n}} \\ &= \left\{ mc^2 \left(1 - \frac{\alpha_{\rm s}^2}{2n^2} \right) \right\}_{n\in\mathbb{N}} + mc^2 O(\alpha_{\rm s}^4),\end{aligned} \tag{2}$$

where $\kappa = j + 1/2$, with $j \in \{1/2, \dots, n - 1/2\}$ being nowadays total angular momentum quantum number.[3] In (2), the expansion of the discrete spectrum in powers of Sommerfeld's fine structure constant $\alpha_{\rm s} = e^2/(\hbar c) \approx 1/137.036$ reminds us that, except for the constant shift[4] by the electron's rest energy mc^2, special relativity only makes tiny corrections $mc^2 \times O(\alpha_{\rm s}^4)$ to the Born–Oppenheimer approximation $m_{\rm p} \to \infty$ of Bohr's energy spectrum

$$\sigma_{\rm pp}^{\rm Bohr} = \left\{ -\frac{\mu c^2 \alpha_{\rm s}^2}{2n^2} \right\}_{n\in\mathbb{N}}; \tag{3}$$

$\mu = m m_{\rm p}/(m + m_{\rm p})$ is the reduced mass of the hydrogen atom, so $\mu \to m$ as $m_{\rm p} \to \infty$.

The Dirac Electron in Reissner–Nordström Spacetime

We next switch on G and ask for the general-relativistic spectrum of a "test" electron in the Reissner–Nordström "electromagnetic spacetime of a point proton." This spacetime is a spherically symmetric, eventually (in an open neighborhood of spacelike infinity) static, charged solution of the Einstein–Maxwell equations (see

[2] We follow the notation of Lieb and Loss [34]; thus $C_c^\infty(\mathbb{R}^3\backslash\{\mathbf{0}\})$ denotes functions which are compactly supported away from the origin in $\mathbb{R}^3$.

[3] For a modern semi-classical approach that produces these quantum numbers, see [30].

[4] The additive constant mc^2 drops out in the calculation of Rydberg's empirical formula for the frequencies of the emitted/absorbed radiation, which are proportional to the differences of the discrete energy eigenvalues.

below), having a metric $\boldsymbol{g}$ with line element $ds_{\boldsymbol{g}}^2 = g_{\mu\nu}dx^\mu dx^\nu$ given by

$$ds_{\boldsymbol{g}}^2 = f(r)c^2dt^2 - f(r)^{-1}dr^2 - r^2(d\theta^2 + \sin^2\theta d\varphi^2), \tag{4}$$

$$f(r) \equiv \left(1 - \frac{2Gm_{\mathrm{p}}}{c^2 r} + \frac{Ge^2}{c^4 r^2}\right); \tag{5}$$

here, (t, r, θ, φ) are Schwarzschild-type coordinates which asymptotically near spacelike infinity become just the spherical coordinates of Minkowski spacetime (obtained by setting $f(r) \equiv 1$ in the above metric). For the empirical values of m_{p} and e, one has $Gm_{\mathrm{p}}^2/e^2 \ll 1$, so this spacetime is then static everywhere and covered by a single chart of (t, r, θ, φ) coordinates, exhibiting a timelike *naked singularity*[5] at $r = 0$.

In the naked singularity sector $Gm_{\mathrm{p}}^2 < e^2$ (recall that the empirical proton's (mass, charge) pair belongs in this sector) one is confronted with the perhaps unexpected result that the Dirac Hamiltonian is not essentially self-adjoint—any general relativist who abhors naked singularities will presumably feel vindicated by this result. Yet, as shown in [5, 8, 16], there exists a one-parameter family of self-adjoint extensions of the Dirac operator with domain $C_c^\infty(\mathbb{R}^3\backslash\{\mathbf{0}\})^4$ which commute with the angular momentum operator, and all of these have an absolutely continuous spectrum given by

$$\sigma_{\mathrm{ac}} = (-\infty, -mc^2] \cup [mc^2, \infty); \tag{6}$$

furthermore, Cohen and Powers [16] show that any pure point spectrum can only be located inside the gap of the continuum. Unfortunately, Cohen and Powers merely state that their preliminary studies indicate the existence of eigenvalues, and we are not aware of any work that has actually shown the existence of eigenvalues for any of the self-adjoint extensions of the formal Dirac operator on the naked Reissner–Nordström spacetime.[6]

[5] This well-known naked singularity is usually not considered to be a counterexample of the (weak) *cosmic censorship hypothesis*, based on the following reasoning: paraphrasing Freeman Dyson, general relativity is a classical physical theory which applies *only to physics in the large* (e.g. astrophysical and cosmic scales), not to atomic physics; and so, since cosmic bodies of mass M and charge Q *must* have a ratio $GM^2/Q^2 \gg 1$, the Reissner–Nordström spacetime of such a body (assumed spherical), when collapsed, exhibits a black hole, not a naked singularity. While we agree that cosmic bodies (in mechanical virial-equilibrium) must have a ratio $GM^2/Q^2 \gg 1$, we don't see why the successful applications of general relativity theory at astrophysical and cosmic scales would imply that general relativity cannot be successfully applied at atomic, or even sub-atomic scales, where typically $GM^2/e^2 \ll 1$.

[6] Interestingly enough, though, Belgiorno–Martellini–Baldicchi [8] proved the existence of bound states of a Dirac point electron *equipped with an anomalous magnetic moment* in the Reissner–Nordström spacetime with naked singularity, provided the anomalous magnetic moment is large enough; in that case, the Dirac Hamiltonian is essentially self-adjoint.

Remark 2.1 One may also want to replace m_{p} by other positive values, in particular by $m_{\mathrm{D}} \approx 2m_{\mathrm{p}}$ (to study the deuterium spectrum) and by $m_{\mathrm{T}} \approx 3m_{\mathrm{p}}$ (to study the tritium spectrum). These choices leave one in the naked-singularity sector of the Reissner–Nordström spacetimes. □

While the general-relativistic hydrogen, deuterium, and tritium problems formulated with the Reissner–Nordström spacetime for an electrostatic point proton inevitably lead to the naked singularity sector, mathematical physicists have also studied a whole family of "hydrogenic problems" with other possible positive mass values M in place of m_{p}. When $G\mathrm{M}^2 \geq e^2$, the analytical extension of the outer Reissner–Nordström spacetime will feature the *event horizon* of a *black hole* behind which lurks the timelike singularity. Moreover, when $G\mathrm{M}^2 > e^2$ then there exists yet another, inner horizon between the timelike singularity and the event horizon, and the region between this and the event horizon is not static. Furthermore, the maximal analytical extension features multiple copies of these spacetime patches, which to some extent are causally separated by *Cauchy horizons*.

For the black hole sector $G\mathrm{M}^2 > e^2$ of parameter space Cohen and Powers [16] showed that the Dirac Hamiltonian is essentially self-adjoint on the set of C^∞ bispinor-valued functions which are compactly supported outside the event horizon, but its spectrum is the *whole real line*, and the pure point spectrum is empty. The problem was picked up again by Belgiorno [5] and by Finster et al. [19], who also proved the absence of bound states supported outside the outer event horizon in the Reissner–Nordström black hole spacetime. The latter authors considered also bispinor wave functions which are supported on both sides of the event horizon; in particular, they also showed that in the extreme case $G\mathrm{M}^2 = e^2$ any bound state must be supported entirely behind the event horizon. An interesting open question is whether in the subextreme black hole sector $G\mathrm{M}^2 > e^2$ any bound state of a self-adjoint Dirac operator must be supported entirely inside the event horizon.

Now, according to the mainstream view of relativists, only the black hole sector of a spacetime family is physically relevant, and for physicists taking the (for a long time also mainstream) positivistic view only the part outside of the black hole's event horizon is of concern to physics—*this combination of viewpoints thus forces one to conclude that in such a physical Reissner–Nordström spacetime there are no bound states of a Dirac point electron without anomalous magnetic moment.*

But positivism is just a form of philosophy, not universally shared by all physicists. And so, if with Werner Israel one believes—as we do—that general relativity makes statements about the *physics* inside the event horizon of a black hole, and explores mathematically what it says the physics is, then *bound states of a Dirac point electron without anomalous magnetic moment may conceivably exist in a physical Reissner–Nordström black hole spacetime, namely supported inside the event horizon.* In the same vein we may as well ignore the censorship hypothesis for the naked-singularity spacetimes and worry about whether *bound states of a Dirac point electron without anomalous magnetic moment exist in a Reissner–Nordström*

spacetime with naked singularity. In either case their existence would yet have to be proved.

But one thing seems clear: none of these putative point spectra can be obtained perturbatively from Sommerfeld's fine structure spectrum by "switching on G." In particular, the black hole point spectrum would presumably vanish as $G \to 0$ because the black hole itself vanishes in this limit, and so bear no resemblance to Sommerfeld's fine structure spectrum as $G \to 0$. And whether any part of any of the hypothetical point spectra for the naked singularity sector will resemble Sommerfeld's fine structure spectrum as $G \to 0$ is anybody's best guess. Hopefully someone will work it out eventually!

Remark 2.2 The putative failure of G-perturbative reasoning can be traced to the non-integrable electromagnetic stresses and energy density which are the source terms for the Ricci curvature tensor of the Reissner–Nordström spacetime. This is the old problem of infinite electrostatic self-energy of a point charge, which because of the equivalence of energy and mass becomes its infinite self-mass problem. In a special-relativistic setting it assigns an infinite inertia to a point charge, which hounds one when trying to formulate a dynamical theory of charged point particle motion beyond the test particle approximation, but in a general-relativistic setting the gravitational coupling leads, in addition, to very strong curvature singularities of the spacetime generated by the non-integrable self-energy densities. Interestingly enough, for the remarkably accurate computation of the special-relativistic quantum-mechanical point spectrum of hydrogen (in the Born–Oppenheimer approximation) only the electrostatic interaction energy of a point proton and a point electron enters the Dirac equation through the usual "minimal coupling," i.e. both self-energy terms are ignored. These self-energy terms are also ignored in the electromagnetic minimal coupling term of Dirac's equation on a Reissner–Nordström spacetime. But the electric self-energy density of the point proton enters the general-relativistic Dirac equation of a point electron in the Reissner–Nordström spacetime also through the covariant derivatives of the spacetime, for this non-integrable density is a curvature source term in the Einstein–Maxwell equations. So one may contemplate purging it, too. This leads to the vacuum Einstein equations, and so instead of the Reissner–Nordström spacetime one would obtain the Schwarzschild spacetime; see [27] for a recent pedagogical treatment. Yet to retain the electrostatic interaction between point electron and proton in the Dirac Hamiltonian, consistent with this approximation, one would next have to solve the Maxwell equations with a point proton as source in a Schwarzschild background spacetime, with the point proton located in its "center"—if this makes any sense at all—and then treat the Dirac point electron as a test charge experiencing the uncharged background metric as well as the electric field of the point proton imposed on that background metric. We are not aware of any such study; furthermore, we are not sure whether a mathematically well-posed formulation of the indicated classical electrical problem is feasible because

the Schwarzschild black hole spacetime is not static inside its event horizon, and its singularity is spacelike, so that its "center" is a spacelike line, not a point, raising the question where exactly to place the point proton! Yet it may be mathematically interesting to sort this out. □

We close this subsection by emphasizing that the just contemplated removal of the self-energy density of the point proton from the spacetime equations is a rather contrived step and not easily justifiable—if at all—, in contrast to the readily vindicated omission of the infinite *self-interaction* terms from the *electromagnetic energy* in the Hamiltonian. It has the flavor of "a last desperate attempt" to cling to the point proton approximation when setting up the general-relativistic hydrogen problem for a Dirac "test electron" interacting with it. Since a physical proton is a compound particle with a finite size, the mathematical catastrophes associated with the point proton approximation may well be dismissed as the result of an oversimplification and declared not a cause for real concern. Indeed, since it is known that finite-size proton models remove the special-relativistic catastrophe of the hydrogenic problem at $Z = 1/\alpha_S \approx 137.036$ [26], it is not difficult to convince oneself that a finite-size model of a spherical proton avoids the general-relativistic spacetime singularity of the Reissner–Nordström spacetime of a point proton. Although this introduces the problem of having to make assumptions about the structure of the proton, the tiny size of the proton suggests that all possible spherical finite size models should yield the same leading order corrections (in terms of powers of G) to the special-relativistic spectrum. For example, assuming a model that produces a spherical surface charge, and zero binding energy, one would obtain a spacetime which coincides with the Reissner–Nordström spacetime for $r > r_p$, and which is flat for $r < r_p$. Here, r_p is the solution to $m_p c^2 - e^2/r = 0$, viz. $r_p = e^2/(m_p c^2)$, which is $\approx$1836 times smaller than the so-called "classical electron radius" $e^2/(mc^2)$, where m is the electron's empirical mass. The spacetime is not smooth at r_p but its singularity corresponds to just a jump in its Ricci curvatures. So a G-perturbative calculation of the Dirac spectrum should be feasible.

2.2 The Hyperfine Structure

So far we have assumed that the proton has only an electric charge. However, the physical proton appears to also possess a magnetic dipole moment. The interaction of the electron spin-magnetic moment with this magnetic moment of the proton accounts for a hyperfine structure of the hydrogen spectrum, as computed with quantum-mechanical perturbation theory. Unfortunately, assuming a point proton carrying an electric charge and magnetic dipole is QM-non-perturbatively catastrophic even in a non-relativistic setting. A QM-non-perturbative calculation requires a model of a finite-size proton. Pekeris [41] proposed that as a substitute for such a finite-size model of the proton with charge and currents one may want to

take the well-known electromagnetic Kerr–Newman spacetime family with its ring singularity and electromagnetic fields which, near spacelike infinity, approach an electric monopole and a magnetic dipole structure. Of course, this proposal should not be taken too seriously, in the sense that the inner structure of the proton is hardly reproduced correctly by the Kerr–Newman solution. Yet it is certainly interesting to investigate Dirac's equation for a point electron in the Kerr–Newman spacetime with its parameters matched to those of the proton.

The Dirac Electron in the Kerr–Newman Spacetime with $G > 0$

In the spirit of the previous subsection we now inquire into the general-relativistic spectrum of a "test" electron in the electromagnetic Kerr–Newman spacetime [38], pretending that its electromagnetic fields represent those of an extended proton with charge and magnetic moment. We do not display its metric (the line element of which is much more complicated than (4); a special case will be exhibited further below, though) but only mention that it has three parameters—charge Q (here chosen to equal e), ADM mass M (here chosen to equal m_p), and ADM angular momentum per unit mass a, here to be chosen such that ea equals the magnetic moment of the proton. This puts us into the naked singularity sector, but as before, we give a mini-survey of both, naked singularity sector and black hole sector, cf. [11].

- The open black hole sector, $G\mathrm{M}^2 > \mathrm{Q}^2 + a^2c^4/G$, was studied in [7, 20, 21, 51], and no bound states of the Dirac equation were found for its domain supported either outside the event horizon or on both sides of it[7]; the latter situation was studied only in [20, 21], involving also a matching across the Cauchy horizon lurking inside the event horizon.
- Interestingly, in the extreme case $G\mathrm{M}^2 = \mathrm{Q}^2 + a^2c^4/G$ (the boundary of the open Kerr-Newman black hole sector, which belongs to the black hole sector, too), bound states supported outside the event horizon exist for a sequence of special m values [51].
- In the naked singularity sector, $G\mathrm{M}^2 < \mathrm{Q}^2 + a^2c^4/G$, the whole spacetime manifold is causally vicious, and we are not aware of any study of the Dirac equation on it.

Since in this subsection we inquire into whether a G-deformation of the Sommerfeld spectrum with hyperfine corrections can be computed by studying Dirac's equation on the Kerr–Newman spacetime, the outcome is somewhat disappointing: the proton parameters $\mathrm{M} = m_\mathrm{p}$ and $\mathrm{Q} = e$ belong to the naked singularity sector of the Kerr–Newman family, and nothing seems to be known about the Dirac equation on it.

On the other hand, since the proton mass does not enter the Sommerfeld fine structure formula, one may still ask about the G-dependence of the discrete Dirac spectra in the extreme Kerr–Newman black hole spacetime and whether

[7] The addition of a positive cosmological constant [6] has not lead to bound states either.

they resemble the Sommerfeld spectrum with hyperfine corrections as $G \to 0$; unfortunately, so far not much is known about these point spectra, either, but someone should work out the answer eventually!

The Dirac Electron in the Zero-*G* Kerr–Newman Spacetime

The inquiry started in the previous subsection suggests a closely related spectral question about the Dirac operator and the Kerr–Newman spacetime, one which avoids all the causal pathologies associated with the latter. Namely, since the canonical (in the sense of Geroch [25]) zero-G limit of the maximal analytically extended Kerr–Newman spacetime (zGKN) does *not* yield the Minkowski spacetime but a flat yet topologically nontrivial spacetime with a ring singularity [47], it is an interesting question whether the Dirac spectrum for an electron in this spacetime bears any resemblance to the Sommerfeld spectrum with hyperfine corrections.

The apparently first investigation in this direction is by Pekeris [41]. However, following Israel [28], he works with the zero-G limit of a *single sheet* of the Kerr–Newman electromagnetic spacetime, which is a Minkowski spacetime decorated with truncated multi-valued harmonic fields. Figure 1, produced by J. Gair and published in [24], and in [35] by D. Lynden-Bell, and which is reproduced here with permission from both D. Lynden-Bell and J. Gair, shows a drawing of electric (top) and magnetic (bottom) lines of force in a planar section, containing the axis of symmetry, of a spacelike snapshot. The ring singularity pierces the drawing at the two singular points where all the field lines seem to emerge from, respectively end at.

If one chooses to interpret the zero-G limit of the spacetime in this single-sheeted way, then one is forced to interpret the inevitable jump discontinuities in the electromagnetic fields as being caused by ultra-singular two-dimensional sources. A geometrically distinguished choice of such a source is the ultra-singular disc source spanned by the ring singularity, studied by [24, 28, 35, 41], and [29]. These disc-type charge and current densities are not integrable, but are magically compensated in parts by oppositely infinite charges and currents on the ring, in such a manner that the finite charge of the Kerr–Newman fields is produced.

By contrast, from the perspective of a two-sheeted interpretation of the zGKN spacetime and its electromagnetic fields the jump discontinuities across the line spanned by the two singular points seen in Fig. 1 are artifacts of the *single-sheeted drawing* of the multi-valued harmonic functions with branch cut placed arbitrarily at the disc spanned by the singular ring. Namely, the sources of the fields living on the double-sheeted maximal analytically extended zero-G Kerr–Newman spacetime are finite sesqui-poles concentrated in the singular ring, see [47]. Thus the Dirac equation on this maximal analytically extended zero-G Kerr–Newman spacetime can be studied in an orderly manner. We have begun such an investigation [31, 32] of Dirac's equation on the maximal analytically extended zero-G Kerr–Newman spacetime, and in the following we report on it.

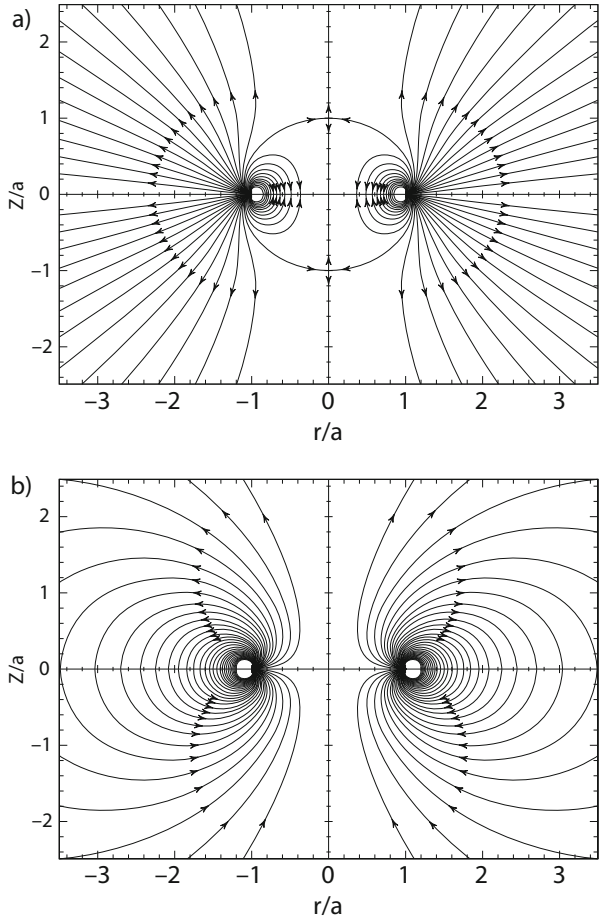


Fig. 1 (From [24] and [35]) Electric (*top*) and magnetic (*bottom*) lines of force in a Euclidean plane containing the (z-)axis of symmetry of a constant-t section of a *single sheet* of the zGKN spacetime; note that in these plots, r denotes a Cartesian coordinate $\perp z$, and not the radial Boyer–Lindquist coordinate! The orientation of the lines (indicated by the *arrows*) reverses across the straight line segment between the two singular points (which are located at $(r/a, z/a) = (-1, 0)$ and $(r/a, z/a) = (1, 0)$); associated with this reversal is a jump discontinuity in the magnitudes of the respective field strengths when one crosses that line segment

In the zero-G limit of the maximal analytically extended Kerr–Newman spacetime with metric expressed in Boyer–Lindquist coordinates (t, r, θ, φ), one obtains a flat double-sheeted spacetime $\mathcal{M}$ with Zipoy topology [54], having a metric $\boldsymbol{g}$ with line element $ds_{\boldsymbol{g}}^2 = g_{\mu\nu} dx^\mu dx^\nu$ given by

$$ds_{\boldsymbol{g}}^2 = c^2 dt^2 - \frac{r^2 + a^2 \cos^2\theta}{r^2 + a^2}(dr^2 + (r^2 + a^2)d\theta^2) - (r^2 + a^2)\sin^2\theta d\varphi^2; \qquad (7)$$

here, $-\infty < t < \infty$, $-\infty < r < \infty$, $0 \leq \theta \leq \pi$, $0 \leq \varphi < 2\pi$. By $\mathcal{N}$ we denote any of the spacelike $t = $ const. slices of the zGKN spacetime $\mathcal{M}$; note that $\mathcal{N}$ is independent of t. The zGKN electromagnetic field is an exact two-form, $\boldsymbol{F} = d\boldsymbol{A}$, with

$$\boldsymbol{A} = -\frac{r}{r^2 + a^2\cos^2\theta}(\mathrm{Q}cdt - \mathrm{Q}a\sin^2\theta d\varphi). \tag{8}$$

We have studied the Dirac Hamiltonian for an electron in the above electromagnetic spacetime. An informal summary of our main results follows:

- The Dirac operator with domain $C_c^\infty(\mathcal{N}, \mathbb{C})^4$ is essentially self-adjoint.
- Its unique self-adjoint extension has a symmetric spectrum about zero.
- Its continuous spectrum is given by $\sigma_{ac} = (-\infty, -mc^2] \cup [mc^2, \infty)$.
- Its discrete spectrum is non-empty if $2|a|mc/\hbar < 1$ and in addition

$$|e\mathrm{Q}|/(\hbar c) < \sqrt{(2|a|mc/\hbar)(1 - 2|a|mc/\hbar)},$$

  and located inside $(-mc^2, mc^2)$.
- If the limit $a \to 0$ of the discrete spectrum converges to the spectrum of the Dirac Hamiltonian on the $a \to 0$ electromagnetic spacetime, it is a union of a positive and a negative Sommerfeld fine structure spectrum.

Remark 2.3 Our sufficient conditions for the existence of the discrete spectrum presumably are not necessary conditions. In any event, for our inquiry into general-relativistic effects on the hydrogen spectrum we use the empirical magnetic moment of the proton and find $2a \approx 10^{-3}\hbar/(mc)$ (in rough agreement with the empirical size of the proton; cf. [41]), so the first sufficient smallness condition is fulfilled (note that it demands that the ring diameter $2|a|$ is smaller than the electron's Compton wavelength $\hbar/(mc)$). And for $\mathrm{Q} = e$ the l.h.s. of the second sufficient smallness condition becomes $\alpha_{\mathrm{s}} \approx 1/137.036$, so the second condition is fulfilled then, too. □

3 A Zero-*G* Kerr-Newman Born-Oppenheimer Hydrogen Atom

In this section we present the essentials of our study. We begin by describing the zero-G Kerr–Newman spacetime and its electromagnetic field in more detail. Then we formulate Dirac's equation on it in its "standard" format, using Cartan's frame method, which allows us to define the Dirac Hamiltonian on a static, spacelike slice of the zGKN spacetime. Finally, we state precisely our results, together with a few remarks regarding our proofs.

3.1 The Zero-Gravity Spacetimes and Their Electromagnetic Fields

The Einstein–Maxwell Equations

An electromagnetic spacetime is a triple $(\mathcal{M}, \boldsymbol{g}, \boldsymbol{F})$, where $(\mathcal{M}, \boldsymbol{g})$ is a four-dimensional Lorentz manifold with metric $\boldsymbol{g}$, and $\boldsymbol{F} = d\boldsymbol{A}$ is the Faraday tensor of the electromagnetic field on $\mathcal{M}$. The Einstein–Maxwell equations for an electromagnetic spacetime are a system of PDEs given by Einstein's field equations

$$R_{\mu\nu}[\boldsymbol{g}] - \frac{1}{2} R g_{\mu\nu} = \frac{8\pi G}{c^4} T_{\mu\nu}[\boldsymbol{F}, \boldsymbol{g}], \tag{9}$$

with $\mu, \nu \in \{0, 1, 2, 3\}$, and where

$$T_{\mu\nu}[\boldsymbol{F}, \boldsymbol{g}] = \frac{1}{4\pi} \left(F^{\lambda}_{\mu} F_{\nu\lambda} - g_{\mu\nu} F_{\alpha\beta} F^{\alpha\beta} \right) \tag{10}$$

is the energy(-density)-momentum(-density)-stress tensor of the electromagnetic field $\boldsymbol{F}$. The Bianchi identities $\nabla^{\mu}(R_{\mu\nu}[\boldsymbol{g}] - \frac{1}{2} R g_{\mu\nu}) = 0$ imply the conservation laws

$$\nabla^{\mu} T_{\mu\nu} = 0, \tag{11}$$

which in turn imply that the Maxwell tensor $\boldsymbol{M} = \star \boldsymbol{F}$ satisfies $d\boldsymbol{M} = 0$; here, $\star$ is the Hodge dual operator. Recall that $d\boldsymbol{F} = 0$ because $dd\boldsymbol{A} = 0$. Incidentally, the Einstein–Maxwell equations simplify somewhat due to the vanishing trace $T^{\mu}_{\mu}(\boldsymbol{F}, \boldsymbol{g}) = 0$, which implies $R = 0$.

The Zero-G Kerr–Newman Spacetime and Its Electromagnetic Field

The Kerr–Newman spacetime with its electromagnetic field is an axisymmetric, asymptotically flat and stationary, three-parameter solution of the above Einstein–Maxwell equations; see [11, 38]. In the limit $G \to 0$ their spacetime metric becomes (7), solving Einstein's vacuum equations $R_{\mu\nu} = 0$ — usually obtained by setting $T_{\mu\nu} \equiv 0$ — while their electromagnetic field $\boldsymbol{F} = d\boldsymbol{A}$, with $\boldsymbol{A}$ given by (8) solves the zero-G Maxwell equations (which in our compact notation look unchanged) on the limiting zero-G spacetime.

The zGKN spacetime is readily illustrated as follows. Since it is static, it suffices to discuss a constant-t snapshot, $\mathcal{N}$, whose metric is given by the space part of (7), with (r, θ, φ) oblate spheroidal coordinates. Since $\mathcal{N}$ is axisymmetric, it furthermore suffices to discuss a constant-φ section of $\mathcal{N}$. Shown in Fig. 2 are the ring singularity and the part $\{r \in (-1, 1), \theta \in (0, \pi)\}$ of such a constant-azimuth

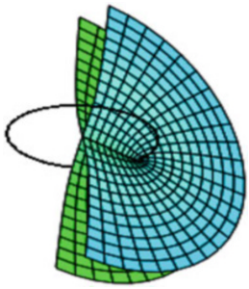


Fig. 2 An illustration of the Zipoy topology

section of $\mathcal{N}$ (slightly curved to separate the sheets for the purpose of visualization); the coordinate grid on the sheets shows the constant-θ lines (hyperbolas) and constant-r lines (ellipses). Solutions to Einstein's equations having this two-sheeted topology were first discovered by Zipoy [54], for which reason we speak of Zipoy topology.

To illustrate the zGKN electromagnetic field, we consider $\boldsymbol{E}+i\boldsymbol{B} = \mathbf{i}_{\partial_t}(\boldsymbol{F}+i\star\boldsymbol{F})$, where $\boldsymbol{E}$ and $\boldsymbol{B}$ are the electric and magnetic fields, obtaining

$$\boldsymbol{E} + i\boldsymbol{B} = -d\frac{\mathrm{Q}}{r - ia\cos\theta}. \tag{12}$$

They were discovered in this form by Appell [1] who realized that these are multi-valued harmonic fields on Euclidean space. The insight that multi-valued harmonic fields become single-valued on so-called *branched Riemann spaces* is due to Sommerfeld [43], whose pioneering work was generalized and completed by Evans [17] and his students. In particular, the fields $\boldsymbol{E}$ and $\boldsymbol{B}$ given in (12) are single-valued harmonic fields on $\mathcal{N}$. Moreover, due to the axisymmetry, the lines of force of $\boldsymbol{E}$ and $\boldsymbol{B}$ are planar curves in doubled half-planes with Zipoy topology which contain the axis of symmetry.

As an illustration of the single-valuedness, and smoothness (except for their divergence at the ring singularity) of the electromagnetic fields on the maximal analytically extended zGKN spacetime, in Fig. 3 we show the graph of the electric potential modulated onto the constant-(t,φ) section of spacetime depicted in Fig. 2. The electric potential is positive on the upper and negative on the lower sheet, diverging at the ring singularity (omitted in this picture, yet discernible due to the spikes in the potential), and smoothly "criss-crossing" at the disc spanned by the singular ring (a line in this constant-(t,φ) section). The electric lines of force (not shown in Fig. 3) are orthogonal to the equipotentials.

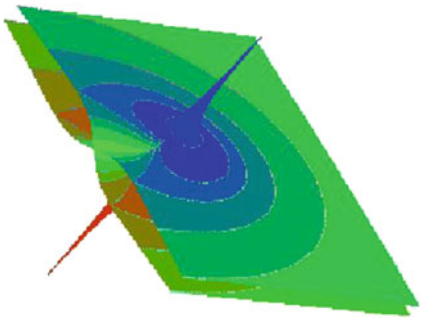


Fig. 3 Graph of the electric potential modulated onto a constant-(t, φ) section of the z*G*KN spacetime. The two sheets are separated and bend for purposes of visualization

3.2 Relativistic Quantum Mechanics in ZGKN Spacetime

The General-Relativistic Dirac Equation

The Dirac equation for a test electron of charge $-e$ and mass m in an electromagnetic Lorentz manifold is a first-order system of PDEs for a bispinor field $\Psi : (\mathcal{M}, \boldsymbol{g}, \boldsymbol{F}) \to \mathbb{C}^4$ given by

$$\tilde{\gamma}^{\mu}(-i\hbar\nabla_{\mu} + \tfrac{1}{c}eA_{\mu})\Psi + mc\Psi = 0; \tag{13}$$

here, the A_{μ} are defined by $\boldsymbol{A} = A_{\mu}dx^{\mu}$, and the $\tilde{\gamma}^{\mu}$ are 4×4 Dirac matrices satisfying the fundamental identity of a Clifford algebra,

$$\tilde{\gamma}^{\mu}\tilde{\gamma}^{\nu} + \tilde{\gamma}^{\nu}\tilde{\gamma}^{\mu} = 2g^{\mu\nu}\mathbf{1}_{4\times 4}, \tag{14}$$

where $(g^{\mu\nu})$ is the inverse matrix to $(g_{\mu\nu})$. Moreover, ∇_{μ} denotes the covariant derivative for the metric $\boldsymbol{g}$.

Dirac's Equation in Standard Form

While concise, the above version of Dirac's equation is not necessarily convenient for analytical studies. It is more convenient to use Cartan's frame formulation [10], which expresses the $\tilde{\gamma}$ matrices in terms of the standard γ matrices of Minkowski spacetime, thus

$$\tilde{\gamma}^{\mu}\nabla_{\mu} = \gamma^{\mu}\boldsymbol{e}_{\mu} + \frac{1}{4}\Omega_{\mu\nu\lambda}\gamma^{\lambda}\gamma^{\mu}\gamma^{\nu}; \tag{15}$$

here we introduced Dirac's gamma matrices, satisfying

$$\gamma^{\nu}\gamma^{\mu} + \gamma^{\mu}\gamma^{\nu} = 2\eta^{\mu\nu}\mathbf{1}_{4\times 4}, \tag{16}$$

where

$$\boldsymbol{\eta} = \mathrm{diag}(1, -1, -1, -1) \tag{17}$$

is the matrix of the Minkowski metric in rectangular coordinates, and we also introduced the Ricci rotation coefficients $\Omega^{\mu}_{\nu\lambda}$ defined by

$$d\boldsymbol{e}^{\mu} = \Omega^{\mu}_{\nu\lambda}\boldsymbol{e}^{\lambda} \wedge \boldsymbol{e}^{\nu} \tag{18}$$

plus an anti-symmetry condition in the lower two parameters; moreover, we introduced the orthonormal frame field

$$(\boldsymbol{e}_{\mu})^{\nu}(\boldsymbol{e}_{\lambda})^{\kappa} g_{\nu\kappa} = \eta_{\mu\lambda}. \tag{19}$$

Finally, we obtain Dirac's equation in standard form (temporarily setting $\hbar = 1 = c$),

$$\gamma^{\mu}\left(\boldsymbol{e}_{\mu} + \Gamma_{\mu} + ie\tilde{A}_{\mu}\right)\Psi + im\Psi = 0, \qquad \Gamma_{\mu} := \frac{1}{4}\Omega_{\nu\lambda\mu}\gamma^{\nu}\gamma^{\lambda}; \tag{20}$$

here

$$\tilde{A}_{\mu} := (\boldsymbol{e}_{\mu})^{\nu} A_{\nu}. \tag{21}$$

The Standard Form of Dirac's Equation on Z*G*KN

We begin by introducing a Cartan (co-)frame $(\boldsymbol{\omega}^{\mu})_{\mu=0,\ldots,3}$ for the cotangent bundle [13]:

$$\begin{aligned} \boldsymbol{\omega}^{0} &:= \frac{\varpi}{|\rho|}(dt - a\sin^2\theta\, d\varphi), \quad \boldsymbol{\omega}^{1} := |\rho| d\theta \\ \boldsymbol{\omega}^{2} &:= \frac{\sin\theta}{|\rho|}(-a dt + \varpi^2 d\varphi), \quad \boldsymbol{\omega}^{3} := \frac{|\rho|}{\varpi} dr, \end{aligned} \tag{22}$$

with the abbreviations

$$\varpi := \sqrt{r^2 + a^2}, \quad \rho := r + ia\cos\theta. \tag{23}$$

Let us denote the oblate spheroidal coordinates (t, r, θ, φ) collectively by (y^{ν}). Let $g_{\mu\nu}$ denote the coefficients of the z*G*KN spacetime metric in oblate spheroidal coordinates, i.e. $g_{\mu\nu} = \boldsymbol{g}\left(\frac{\partial}{\partial y^{\mu}}, \frac{\partial}{\partial y^{\nu}}\right)$. One easily checks that written in the $(\boldsymbol{\omega}^{\mu})$ frame, the spacetime line element is

$$ds^2_{\boldsymbol{g}} = g_{\mu\nu} dy^{\mu} dy^{\nu} = \eta_{\alpha\beta}\boldsymbol{\omega}^{\alpha}\boldsymbol{\omega}^{\beta}. \tag{24}$$

With respect to this frame the electromagnetic Sommerfeld potential $\boldsymbol{A} = \tilde{A}_\mu \boldsymbol{\omega}^\mu$, with

$$\tilde{A}_0 = -\mathrm{Q}\,\frac{r}{|\rho|\varpi}, \quad \tilde{A}_1 = 0, \quad \tilde{A}_2 = 0, \quad \tilde{A}_3 = 0. \tag{25}$$

The frame of vector fields $(\boldsymbol{e}_\mu)$ is the *dual* frame to $(\boldsymbol{\omega}^\mu)$, yielding an orthonormal basis for the tangent space at each point in the manifold:

$$\begin{aligned} \boldsymbol{e}_0 &= \frac{\varpi}{|\rho|}\partial_t + \frac{a}{\varpi|\rho|}\partial_\varphi, \quad \boldsymbol{e}_1 = \frac{1}{|\rho|}\partial_\theta \\ \boldsymbol{e}_2 &= \frac{a\sin\theta}{|\rho|}\partial_t + \frac{1}{|\rho|\sin\theta}\partial_\varphi, \quad \boldsymbol{e}_3 = \frac{\varpi}{|\rho|}\partial_r\,. \end{aligned} \tag{26}$$

Next, the anti-symmetric matrix $\left(\Omega_{\mu\nu}\right) = \left(\eta_{\mu\lambda}\Omega^\lambda_\nu\right)$ is computed to be

$$(\Omega_{\mu\nu}) = \begin{pmatrix} 0 & -C\boldsymbol{\omega}^0 - D\boldsymbol{\omega}^2 & D\boldsymbol{\omega}^1 - B\boldsymbol{\omega}^3 & -A\boldsymbol{\omega}^0 - B\boldsymbol{\omega}^2 \\ & 0 & D\boldsymbol{\omega}^0 + F\boldsymbol{\omega}^2 & -E\boldsymbol{\omega}^1 - C\boldsymbol{\omega}^3 \\ & (\text{anti-sym}) & 0 & -B\boldsymbol{\omega}^0 - E\boldsymbol{\omega}^2 \\ & & & 0 \end{pmatrix}, \tag{27}$$

where

$$A := \frac{a^2 r\sin^2\theta}{\varpi|\rho|^3},\ B := \frac{ar\sin\theta}{|\rho|^3},\ C := \frac{a^2\sin\theta\cos\theta}{|\rho|^3}, \tag{28}$$

$$D := \frac{a\cos\theta\,\varpi}{|\rho|^3},\ E := \frac{r\varpi}{|\rho|^3},\ F := \frac{\varpi^2\cos\theta}{|\rho|^3\sin\theta}. \tag{29}$$

With respect to this frame on a z*G*KN spacetime the covariant derivative part of the Dirac operator can be expressed with the help of the operator

$$\mathfrak{O} := \tilde{\gamma}^\mu\nabla_\mu = \begin{pmatrix} 0 & \mathfrak{l}' + \mathfrak{m}' \\ \mathfrak{l} + \mathfrak{m} & 0 \end{pmatrix}, \tag{30}$$

where

$$\mathfrak{l} := \frac{1}{|\rho|}\begin{pmatrix} D_+ & L_- \\ L_+ & D_- \end{pmatrix} \tag{31}$$

and

$$\mathfrak{l}' := \frac{1}{|\rho|}\begin{pmatrix} D_- & -L_- \\ -L_+ & D_+ \end{pmatrix}, \tag{32}$$

with

$$D_\pm := \pm\varpi\,\partial_r + \varpi\,\partial_t + \frac{a}{\varpi}\partial_\varphi, \quad L_\pm := \partial_\theta \pm i\left(a\sin\theta\,\partial_t + \csc\theta\partial_\varphi\right), \tag{33}$$

while (with * denoting complex conjugation)

$$\begin{aligned}\mathfrak{m} &:= \frac{1}{2}\big[(-2C + F + iB)\sigma_1 + (-A + 2E + iD)\sigma_3\big] \\ &= \frac{1}{2|\rho|}\begin{pmatrix} \frac{r}{\varpi} + \frac{\varpi}{\rho^*} & \cot\theta + \frac{ia\sin\theta}{\rho^*} \\ \cot\theta + \frac{ia\sin\theta}{\rho^*} & -\frac{r}{\varpi} - \frac{\varpi}{\rho^*}\end{pmatrix}\end{aligned} \tag{34}$$

and

$$\mathfrak{m}' := \frac{1}{2}\big[(2C - F + iB)\sigma_1 + (A - 2E + iD)\sigma_3\big] = -\mathfrak{m}^\dagger, \tag{35}$$

where † denotes the Hermitian adjoint, and where the σ_k are Pauli matrices, viz.

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0\end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0\end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1\end{pmatrix}. \tag{36}$$

The principal part of $|\rho|\mathfrak{O}$ has the separation property

$$\begin{aligned}|\rho|\begin{pmatrix} 0 & \mathfrak{l}' \\ \mathfrak{l} & 0\end{pmatrix} &= \Big[\gamma^3\varpi\,\partial_r + \gamma^0\left(\varpi\,\partial_t + \frac{a}{\varpi}\partial_\varphi\right)\Big] \\ &\quad + \Big[\gamma^1\partial_\theta + \gamma^2(a\sin\theta\partial_t + \csc\theta\,\partial_\varphi)\Big],\end{aligned} \tag{37}$$

where the coefficients of the two square-bracketed operators are functions of only r, respectively only θ, and the lower order term in $\mathfrak{O}$ can be transformed away, achieving exact separation for $|\rho|\mathfrak{O}$. Namely, setting

$$\chi(r,\theta) := \frac{1}{2}\log(\varpi\rho^*\sin\theta), \tag{38}$$

it is easy to see that

$$\mathfrak{m} = \mathfrak{l}\chi, \quad \mathfrak{m}' = \mathfrak{l}'\chi^*. \tag{39}$$

Define now the diagonal matrix

$$\mathfrak{D} := \mathrm{diag}(e^{-\chi}, e^{-\chi}, e^{-\chi^*}, e^{-\chi^*}) \tag{40}$$

and a new bispinor $\hat{\Psi}$ related to the original Ψ by

$$\Psi = \mathfrak{D}\hat{\Psi}, \tag{41}$$

and denoting the upper and lower components of a bispinor Ψ by ψ_1 and ψ_2 respectively, it now follows that

$$(\mathfrak{l} + \mathfrak{m})\psi_1 = (\mathfrak{l} + \mathfrak{m})(e^{-\chi}\hat{\psi}_1) = e^{-\chi}\left[\mathfrak{l} - \mathfrak{l}\chi + \mathfrak{m}\right]\hat{\psi}_1 = e^{-\chi}\mathfrak{l}\hat{\psi}_1, \tag{42}$$

and similarly

$$(\mathfrak{l}' + \mathfrak{m}')\psi_2 = e^{-\chi^*}\mathfrak{l}'\hat{\psi}_2. \tag{43}$$

Setting

$$\mathfrak{R} := \mathrm{diag}(\rho, \rho, \rho^*, \rho^*) \tag{44}$$

and noting that $|\rho|\mathfrak{D}^{-\dagger}\mathfrak{D} = \mathfrak{R}$ while $\mathfrak{D}^{-\dagger}\gamma^\mu\mathfrak{D} = \gamma^\mu$ (where $\mathfrak{D}^{-\dagger}$ is shorthand for $(\mathfrak{D}^{-1})^\dagger$), we insert $\Psi = \mathfrak{D}\hat{\Psi}$ in (20) and left-multiply the equation by the diagonal matrix $\mathfrak{D}' := |\rho|\mathfrak{D}^{-\dagger}$, and conclude that $\hat{\Psi}$ solves the transformed Dirac equation

$$\left(|\rho|\gamma^\mu(\boldsymbol{e}_\mu + ie\tilde{A}_\mu) + im\mathfrak{R}\right)\hat{\Psi} = 0. \tag{45}$$

The Dirac Hamiltonian on a Constant-*t* Snapshot of *ZGKN* Spacetime

We now recast Dirac's equation (45) for Ψ in Schrödinger form,

$$i\hbar\partial_t\hat{\Psi} = \hat{H}\hat{\Psi}, \tag{46}$$

for which we have to compute the Dirac Hamiltonian from (45). Let matrices M^μ be defined by

$$|\rho|\gamma^\mu\boldsymbol{e}_\mu = M^\mu\partial_\mu. \tag{47}$$

In particular,

$$M^0 = \varpi\gamma^0 + a\sin\theta\,\gamma^2. \tag{48}$$

We may thus rewrite (45) as

$$M^0\partial_t\hat{\Psi} = -\left(M^k\partial_k + ie|\rho|\gamma^\mu\tilde{A}_\mu + im\mathfrak{R}\right)\hat{\Psi}. \tag{49}$$

Finally, restoring $\hbar$ and c, and defining

$$\hat{H} := (M^0)^{-1}\left(M^k(-i\hbar\partial_k) + \tfrac{1}{c}e|\rho|\gamma^\mu\tilde{A}_\mu + mc\mathfrak{R}\right), \tag{50}$$

we arrive at (46).

A Hilbert Space for $\hat{H}$

In order to obtain the correct inner product for the space of bispinor fields defined on the zGKN spacetime, we left-multiply the original Dirac equation (13) by the conjugate bispinor $\overline{\Psi}$, defined as

$$\overline{\Psi} := \Psi^\dagger\gamma^0, \tag{51}$$

integrate the result over a slab of spacetime, and obtain the action for this equation. We find

$$\mathcal{S}[\Psi] = \int_I dt \int_{\Sigma_t} \Psi^\dagger\gamma^0\left[\tilde{\gamma}^\mu\nabla_\mu\Psi + \dots\right] d\mu_{\Sigma_t}, \tag{52}$$

where $I \subset \mathbb{R}$ is a finite interval, and $d\mu_{\Sigma_t}$ is the volume element of $\Sigma_t \equiv \mathcal{N}$, any spacelike $t =$ constant slice of the zGKN spacetime. Using oblate spheroidal coordinates, with $d\mu_{\mathcal{N}} = |\rho|^2\sin\theta d\theta d\varphi dr$, it follows that the natural inner product for bispinors on $\Sigma_t = \mathcal{N}$ needs to be

$$\langle\Psi,\Phi\rangle = \int_{\mathcal{N}} \Psi^\dagger\gamma^0\tilde{\gamma}^0\Phi d\mu_{\mathcal{N}} = \int_0^{2\pi}\int_0^{\pi}\int_{-\infty}^{\infty} \Psi^\dagger M\Phi|\rho|^2\sin\theta d\theta d\varphi dr, \tag{53}$$

with

$$M := \gamma^0\tilde{\gamma}^0 = \gamma^0\boldsymbol{e}^0_\nu\gamma^\nu = \frac{\varpi}{|\rho|}\alpha^0 + \frac{a\sin\theta}{|\rho|}\alpha^2. \tag{54}$$

Here, α^2 is the second one of the three Dirac alpha matrices in the Weyl (spinor) representation

$$\alpha^k = \gamma^0\gamma^k = \begin{pmatrix}\sigma_k & 0\\ 0 & -\sigma_k\end{pmatrix}, \qquad k = 1,2,3, \tag{55}$$

and for notational convenience the 4×4 identity matrix has been denoted by

$$\alpha^0 = \begin{pmatrix}\mathbf{1}_{2\times 2} & 0\\ 0 & \mathbf{1}_{2\times 2}\end{pmatrix}. \tag{56}$$

Now, let $\Psi = \mathfrak{D}\hat{\Psi}$ and $\Phi = \mathfrak{D}\hat{\Phi}$, with $\mathfrak{D}$ as in (40). Then we have

$$\langle \Psi, \Phi \rangle = \int_0^{2\pi} \int_0^{\pi} \int_{-\infty}^{\infty} \hat{\Psi}^\dagger \hat{M} \hat{\Phi} d\theta d\varphi dr, \tag{57}$$

where

$$\hat{M} := \alpha^0 + \frac{a \sin\theta}{\varpi} \alpha^2. \tag{58}$$

The eigenvalues of $\hat{M}$ are $\lambda_\pm = 1 \pm a \sin\theta/\varpi$, both of which have multiplicity 2 and are positive everywhere on this space with Zipoy topology. (Note that $\lambda_- \to 0$ on the ring, which is not part of the spacetime but of its boundary.) We may thus take the above as the definition of a positive definite inner product given by the matrix $\hat{M}$ for bispinors defined on any $t =$ constant section of $\mathcal{M}$, a rectangular cylinder $\mathcal{Z} := \mathbb{R} \times [0, \pi] \times [0, 2\pi]$ with its natural measure:

$$\langle \hat{\Psi}, \hat{\Phi} \rangle_{\hat{M}} := \int_{\mathcal{Z}} \hat{\Psi}^\dagger \hat{M} \hat{\Phi} d\theta d\varphi dr. \tag{59}$$

The corresponding Hilbert space is denoted by H, thus

$$\mathsf{H} := \left\{ \hat{\Psi} : \mathcal{Z} \to \mathbb{C}^4 \mid \|\hat{\Psi}\|^2_{\hat{M}} := \langle \hat{\Psi}, \hat{\Psi} \rangle_{\hat{M}} < \infty \right\}. \tag{60}$$

Note that H is *not equivalent* to $L^2(\mathcal{Z})$ whose inner product has the identity matrix in place of $\hat{M}$. We are finally ready to list our main results which are proved in [32].

Symmetry of the Spectrum of $\hat{H}$

Following the strategy of Glazman, in [32] we prove:

Theorem 3.1 *Let any self-adjoint extension of the formal Dirac operator $\hat{H}$ on H be denoted by the same letter. Suppose $E \in \operatorname{spec} \hat{H}$. Then $-E \in \operatorname{spec} \hat{H}$.*

Remark 3.2 We can also replace $\mathrm{Q}a$ with $\mathrm{I}\pi a^2/c$ in (8), introducing a KN-anomalous magnetic moment; here I is an electrical current supported by the ring singularity, independently of Q. This changes $\tilde{A}_0$ and $\tilde{A}_2$ to

$$\tilde{A}_0 = -\mathrm{Q}\frac{r}{|\rho|\varpi} - \left(\mathrm{Q} - \frac{\mathrm{I}\pi a}{c}\right) \frac{a^2 r \sin^2\theta}{\varpi |\rho|^3}, \; \tilde{A}_2 = -\left(\mathrm{Q} - \frac{\mathrm{I}\pi a}{c}\right) \frac{ar \sin\theta}{|\rho|^3}. \tag{61}$$

Our symmetry result Theorem 3.1 holds for *any* self-adjoint extension of $\hat{H}$, whatever Q and I. □

Essential Self-Adjointness of $\hat{H}$

Adapting an argument of Winklmeier–Yamada [51], in [32] we prove:

Theorem 3.3 *Let* $\mathrm{Q} = e = \mathrm{I}\pi a/c$. *Let* $\mathcal{Z}^\circ$ *denote* $\mathcal{Z}$ *with the ring singularity* $\{(r,\theta,\varphi)|r = 0, \theta = \pi/2\}$ *deleted. Then* $\hat{H}$ *with domain* $C_c^\infty(\mathcal{Z}^\circ)$ *is essentially self-adjoint on* H.

The unique self-adjoint extension of $\hat{H}$ will also be denoted by $\hat{H}$.

The Continuous Spectrum of $\hat{H}$

Using the Chandrasekhar–Page–Toop separation of variables, and an argument of Weidmann [50], in [32] we prove:

Theorem 3.4 *For* $\mathrm{Q} = e = \mathrm{I}\pi a/c$, *the continuous spectrum of* $\hat{H}$ *on* H *is* $\mathbb{R} \setminus (-mc^2, mc^2)$.

The Point Spectrum

In [32] we prove:

Theorem 3.5 *Let* $\mathrm{Q} = e = \mathrm{I}\pi a/c$. *If*

$$2|a| < \frac{\hbar}{mc} \quad \text{and} \quad \frac{e^2}{\hbar c} < \sqrt{\frac{2|a|}{\hbar/(mc)}\left(1 - \frac{2|a|}{\hbar/(mc)}\right)},$$

the point spectrum of $\hat{H}$ *on* H *is nonempty and located in* $(-mc^2, mc^2)$; *the end points are not included.*

Remark 3.3 In the *hydrogenic* problem where the "proton" charge e is replaced by the charge $\mathrm{Q} = \mathrm{Z}e$ of a "nucleus," with $\mathrm{Z} > 1$ (and the proton mass m_p by the nuclear mass $\mathrm{M} > 0$ — although this does not show in the zero-G formulation of the problem of a "test" electron in the electromagnetic field of a nucleus), a point spectrum exists in the gap of the continuum as long as $\mathrm{Z} < 137.036\sqrt{\frac{2|a|}{\hbar/(mc)}\left(1 - \frac{2|a|}{\hbar/(mc)}\right)}$. Since our upper bound on Z goes $\searrow 0$ as $|a| \searrow 0$, it is presumably not sharp, at least not when judged against the familiar Dirac bound $\mathrm{Z} < 137.036$ for the existence of a point spectrum in the hydrogenic problem with point nuclei on Minkowski spacetime. □

We briefly indicate our strategy of proof of the point spectrum. We employ the Chandrasekhar–Page–Toop separation of variables ansatz,

$$\Psi(t,r,\theta,\varphi) = e^{-iEt+i\kappa\varphi}\begin{pmatrix} R_1(r)S_1(\theta) \\ R_2(r)S_2(\theta) \\ R_2(r)S_1(\theta) \\ R_1(r)S_2(\theta) \end{pmatrix}, \tag{62}$$

with $E \in (-mc^2, mc^2)$ and $2|\kappa| \in \mathbb{Z} \setminus \{0\}$, obtaining coupled eigenvalue problems for $\vec{R} = (R_1, R_2)^t$ and $\vec{S} = (S_1, S_2)^t$,

$$T_{rad}\vec{R} = E\vec{R}, \qquad T_{ang}\vec{S} = \lambda\vec{S}, \tag{63}$$

where

$$T_{rad} = \begin{pmatrix} i\frac{d}{dr} - \frac{-a\kappa+eQr}{\varpi^2} & -m\frac{r}{\varpi} - i\frac{\lambda}{\varpi} \\ -m\frac{r}{\varpi} + i\frac{\lambda}{\varpi} & -i\frac{d}{dr} - \frac{-a\kappa+eQr}{\varpi^2} \end{pmatrix} \tag{64}$$

and

$$T_{ang} = \begin{pmatrix} -ma\cos\theta & -\frac{d}{d\theta} - \left(aE\sin\theta - \frac{\kappa}{\sin\theta}\right) \\ \frac{d}{d\theta} - \left(aE\sin\theta - \frac{\kappa}{\sin\theta}\right) & ma\cos\theta \end{pmatrix}. \tag{65}$$

The Prüfer transform

$$R_1 = Re^{i\Omega/2},\ R_2 = Re^{-i\Omega/2},\ S_1 = S\cos\frac{\Theta}{2},\ S_2 = S\sin\frac{\Theta}{2} \tag{66}$$

now yields a partly decoupled nonlinear eigenvalue system,

$$\begin{cases} d\Omega/dr = 2\frac{mr}{\varpi}\cos\Omega + 2\frac{\lambda}{\varpi}\sin\Omega + 2\frac{a\kappa+\gamma r}{\varpi^2} - 2E \\ d(\ln R)/dr = \frac{mr}{\varpi}\sin\Omega - \frac{\lambda}{\varpi}\cos\Omega \end{cases} \tag{67}$$

$$\begin{cases} d\Theta/d\theta = 2\left(\lambda - ma\cos\theta\cos\Theta + \left(aE\sin\theta - \frac{\kappa}{\sin\theta}\right)\sin\Theta\right) \\ d(\ln S)/d\theta = -ma\cos\theta\sin\Theta - \left(aE\sin\theta - \frac{\kappa}{\sin\theta}\right)\cos\Theta. \end{cases} \tag{68}$$

Note that in each pair of equations the second one can be integrated once a solution to the first one is known. The first equation in each pair is independent of the second one in the pair; however, the two first equations are still coupled through the eigenvalue parameters and need to be solved jointly.

There are integrability conditions. Combined with the Chandrasekhar et al. ansatz the Prüfer transform yields

$$\Psi(t,r,\theta,\varphi) = R(r)S(\theta)e^{-i(Et-\kappa\varphi)} \begin{pmatrix} \cos(\Theta(\theta)/2)e^{+i\Omega(r)/2} \\ \sin(\Theta(\theta)/2)e^{-i\Omega(r)/2} \\ \cos(\Theta(\theta)/2)e^{-i\Omega(r)/2} \\ \sin(\Theta(\theta)/2)e^{+i\Omega(r)/2} \end{pmatrix}, \tag{69}$$

and $\Psi \in L^2$ iff:

$$\left.\begin{array}{llll} \Omega(-\infty) = & -\pi + \cos^{-1}(E), & \Omega(\infty) = & -\cos^{-1}(E) \\ \Theta(0) = & 0, & \Theta(\pi) = & -\pi. \end{array}\right\} \tag{70}$$

The two coupled Eqs. (67), (68), supplemented by the asymptotic conditions (70), can be interpreted as a dynamical system and now treated as such with dynamical systems theory; for the many details, see [32]. This completes the survey of our main results from [32].

We have also numerically computed (what we believe is) the positive energy ground state for various a values; a typical profile is shown in Fig. 4. For small $|a|$ the profile is close to the known hydrogen ground state profile for $a = 0$ in the $r > 0$ sheet; in addition, a tiny exponentially decaying "tail" extends into the $r < 0$ sheet.

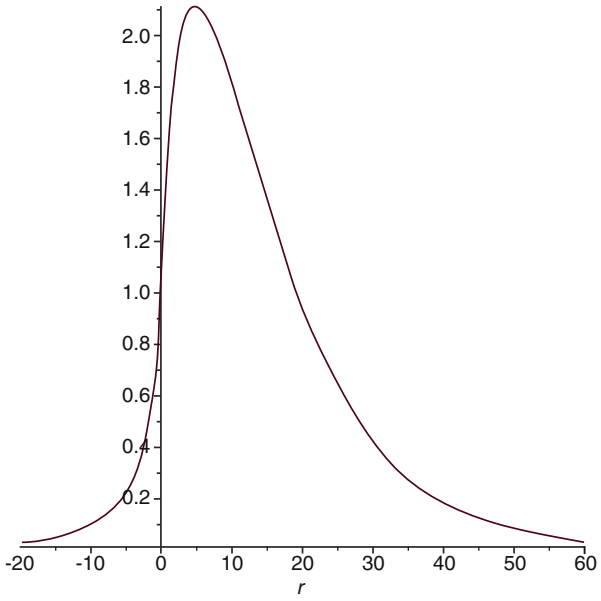


Fig. 4 The square of the absolute (putative) positive ground state versus the oblate spheroidal r coordinate

This is what one would intuitively expect from a negatively charged electron in the $r > 0$ sheet that is attracted to a small-a ring singularity which appears positively charged in the $r > 0$ sheet: the likelihood of finding the electron on the negatively charged side of the ring singularity should be exponentially small. Interestingly, by anti-symmetry, the negative energy "ground" state (in the sense of having smallest absolute energy) is obtained by reflection of the positive energy ground state profile at $r = 0$. By the same kind of "intuitive explanation" given of the behavior of the electron in the positive energy ground state, the negative energy ground state corresponds to the behavior expected rather from a positron.

4 Summary and Outlook

4.1 Summary

Motivated by the mathematical-physics problem of general-relativistic extensions of the Sommerfeld fine-structure spectrum of hydrogen, in particular those including the hyper-fine structure, in this presentation we have addressed the Dirac equation of a point electron in the zero-G limit of the maximal analytically extended, double-sheeted Kerr–Newman spacetime. A related study has been proposed by Pekeris [41] who, however, studied Dirac's equation on a *one-sheeted truncation* of the zGKN spacetime, which comes at the price of nonintegrable "proton" charge and current "densities" concentrated in a disc[8] and raises the question of boundary conditions for the Dirac bispinors at the disc; cf. also [24]. By contrast, we have found that our zGKN Dirac Hamiltonian is essentially self-adjoint, and its unique self-adjoint extension has a spectrum which is symmetric about zero, containing the familiar continuum $(-\infty, -mc^2) \cup (mc^2, \infty)$ plus, under a smallness condition, a discrete spectrum in the gap of the continuum; for the hydrogen parameter values the smallness condition is satisfied. Moreover, our results imply that the point spectrum converges to two anti-symmetric copies of the Sommerfeld spectrum when the ring radius of the zGKN spacetime vanishes, if it converges to the spectrum of the zero-a operator.

We end this summary with a disclaimer: we are not advocating that the ring singularity of the double-sheeted zGKN spacetime were an accurate model for a physical proton. Rather, our zGKN Born–Oppenheimer hydrogen atom model is merely an interesting toy model which reduces to the familiar special-relativistic Born–Oppenheimer hydrogen atom model (and an anti-symmetric copy thereof) when $a = 0$, and thus allows one to rigorously study non-perturbatively some general-relativistic $a > 0$ effects on the quantum-mechanical hydrogen spectrum, such as the hyperfine structure (which cannot be studied non-perturbatively with the point proton model, featuring an electric charge and a magnetic dipole moment).

[8] For integrable yet infinitely extended astrophysical Kerr–Newman disc sources, see [33].

4.2 Outlook

Our study leaves many questions unanswered, but also suggests some intriguing speculations (the latter were not included in the talk at Regensburg).

Open Questions

First of all, we would like to know the point spectrum of the "double-sheeted zGKN" Dirac Hamiltonian in more detail, and as function of the ring radius a; a numerical study is currently in progress.

More in line with PDE research into Dirac's equation on general relativistic spacetimes, we would like to know what happens when a Dirac bispinor wave function impinges on the zGKN ring singularity; in particular, how much of it scatters and how much will dive through the ring?

Furthermore, we would like to know what happens if the zGKN magnetic moment $\mathrm{Q}a$ is replaced by $\mathrm{I}\pi a^2/c$, so that the electromagnetic zGKN spacetime becomes a zGK spacetime decorated with an Appell–Sommerfeld field of arbitrary charge Q and current I. Is the Dirac Hamiltonian still essentially self-adjoint? If not, are there distinguished self-adjoint extensions? Can one characterize the spectrum of the self-adjoint extension(s)? Note that, if $\mathrm{Q} \neq \mathrm{I}\pi a/c$ then the Chandrasekhar–Page–Toop ansatz to separate variables fails, and one is faced with a two-variable PDE eigenvalue problem.

Incidentally, independent of any inquiry into the Dirac equation, the following question is relevant to the problem of uniqueness of the Kerr–Newman manifold: is it possible to G-deform the zGK spacetime decorated with an Appell–Sommerfeld field of charge Q and current I into a solution of the Einstein–Maxwell equations only for the KN choice $\mathrm{Q}a = \mathrm{I}\pi a^2/c$?

Thus we also would like to investigate what happens when gravity is "switched back on." After reviewing the enormous obstacles which are encountered in the pertinent literature on the subject, we concluded that these are caused mainly by the non-integrable electromagnetic self-energy densities of point electron and point or ring proton as computed with the linear Maxwell–Lorentz equations which lead to unphysical spacetime curvatures once gravity is switched on. To avoid these problems we plan to study the nonlinear Einstein–Maxwell–Born–Infeld system, which promises to yield the mildest conceivable spacetime singularities [46]. Unfortunately, their nonlinearity is formidable, and progress will most likely come slowly. Moreover, it is clear that one has to abandon the Born–Oppenheimer approximation, but the full two-body problem (cf. [9]) may still be out of reach.

Speculations

As for the intriguing speculations, our research also led to a completely different line of inquiry which we have embarked on in [31]. Namely, as has been advocated by Stückelberg [44], Feynman [18], Thaller [48, 49], and others, the puzzling spectral properties of Dirac's equation interpreted quantum mechanically, as again highlighted by the mysterious anti-symmetry of the Dirac spectrum of a "point electron" in the anti-symmetric double-sheeted z*G*KN spacetime, suggest that Dirac's equation captures the dynamics and bound states of both *electron and positron*. Yet interpreted as a quantum-mechanical equation, Dirac's equation is a *single particle* equation. This has suggested to us to entertain the hypothesis that particles and anti-particles are merely "different sides of the same medal," i.e. forming a single meta-particle with a binary structure, rather than being different particles in their own right. The very anti-symmetric structure of the z*G*KN ring singularity supplies just such a binary structure, which in [31] we have tentatively identified with an electron/anti-electron meta-particle. There we show that the Dirac spectrum of such a z*G*KN-ring particle in the electrostatic field of a given point charge (now playing the role of the point proton) with straight world line in the pertinent z*G*KN spacetime is determined by the same equation that we have discussed in this presentation. It's the narrative that changes, not the mathematics. This narrative, where electron and anti-electron are just two different "sides of the same medal," is faithfully realized by the electromagnetic ring singularity of the z*G*KN spacetime, and we ponder seriously the possibility of it having a true physical significance.

Acknowledgements Many thanks go to Felix Finster, Jürgen Tolksdorf, and Eberhard Zeidler for their kind invitation to present these results at their superbly organized conference, and for the financial support and the impeccable hospitality offered by the organizers and their staff. We also thank Donald Lynden-Bell and Jonathan Gair for the permission to reproduce their field line drawings (Fig. 1). Finally, we thank the referee for a very careful reading of our paper, and for constructive criticisms.

References

1. P. Appell, Quelques remarques sur la théorie des potentiels multiforms. Math. Ann. **30**, 155–156 (1887)
2. D. Batic, H. Schmid, The Dirac propagator in the Kerr–Newman metric. Prog. Theor. Phys. **116**, 517–544 (2006)
3. D. Batic, H. Schmid, Chandrasekhar Ansatz and the generalized total angular momentum operator for the Dirac equation in the Kerr–Newman metric. Rev. Colomb. Mat. **42**, 183–207 (2008)
4. D. Batic, H. Schmid, M. Winklmeier, On the eigenvalues of the Chandrasekhar-Page angular equation. J. Math. Phys. **46**, 012504 (35) (2005)
5. F. Belgiorno, Massive Dirac fields in naked and in black hole Reissner–Nordström manifolds. Phys. Rev. D **58**, 084017 (8) (1998)

6. F. Belgiorno, S.L. Cacciatori, The Dirac equation in Kerr–Newman–AdS black hole background. J. Math. Phys. **51**, 033517 (32) (2010)
7. F. Belgiorno, M. Martellini, Quantum properties of the electron field in Kerr-Newman black hole manifolds. Phys. Lett. B **453**, 17–22 (1999)
8. F. Belgiorno, M. Martellini, M. Baldicchi, Naked Reissner-Nordström singularities and the anomalous magnetic moment of the electron field. Phys. Rev. D **62**, 084014 (2000)
9. H.A. Bethe, E.E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Plenum Press, New York, 1977)
10. D.R. Brill, J.M. Cohen, Cartan frames and the general relativistic Dirac equation. J. Math. Phys. **7**, 238–243 (1966)
11. B. Carter, Global structure of the Kerr family of gravitational fields. Phys. Rev. **174**, 1559–1571 (1968)
12. A. Cáceres, C. Doran, Minimax determination of the energy spectrum of the Dirac equation in a Schwarzschild background. Phys. Rev. A **72**, 022103(7) (2005)
13. B. Carter, R.G. McLenaghan, Generalized master equations for wave equation separation in a Kerr or Kerr-Newman black hole background, in *Proceedings of the 2nd Marcel Grossmann meeting on general relativity*, ed. by R. Ruffini (North-Holland, Amsterdam, 1982), pp. 575–585
14. S. Chandrasekhar, The solution of Dirac's equation in Kerr geometry. Proc. R. Soc. Lond. Ser. A **349**, 571–575 (1976)
15. S. Chandrasekhar, Errata: the solution of Dirac's equation in Kerr geometry. Proc. R. Soc. Lond. Ser. A **350**, 565 (1976)
16. J.M. Cohen, R.T. Powers, The general relativistic hydrogen atom. Commun. Math. Phys. **86**, 69–86 (1982)
17. G.C. Evans, *Lectures on Multiple-Valued Harmonic Functions in Space* (University of California Press, Berkeley/Los Angeles, 1951)
18. R.P. Feynman, Theory of positrons. Phys. Rev. **76**, 749–759 (1949)
19. F. Finster, J. Smoller, S.-T. Yau, Nonexistence of time-periodic solutions of the Dirac equation in Reissner–Nordström black hole background. J. Math. Phys. **41**, 2173–2194 (2000)
20. F. Finster, N. Kamran, J. Smoller, S.-T. Yau, Nonexistence of time-periodic solutions of the Dirac equation in an axisymmetric black hole geometry. Commun. Pure Appl. Math. **53**, 902–929 (2000)
21. F. Finster, N. Kamran, J. Smoller, S.-T. Yau, Erratum: nonexistence of time-periodic solutions of the Dirac equation in an axisymmetric black hole geometry. Commun. Pure Appl. Math. **53**, 1201 (2000)
22. F. Finster, N. Kamran, J. Smoller, S.-T. Yau, Decay rates and probability estimates for massive Dirac particles in the Kerr–Newman black hole geometry. Commun. Math. Phys. **230**, 201–244 (2002)
23. F. Finster, N. Kamran, J. Smoller, S.-T. Yau, The long-time dynamics of Dirac particles in the Kerr–Newman black hole geometry. Adv. Theor. Math. Phys. **7**, 25–52 (2003)
24. J. Gair, *An Investigation of Bound States in the Kerr–Newman Potential*. Prize Essay (Cambridge University, 2001)
25. R. Geroch, Limits of spacetimes. Commun. Math. Phys. **13**, 180–193 (1969)
26. W. Greiner, B. Müller, J. Rafelski, *Quantum Electrodynamics of Strong Fields* (Springer, Berlin/New York, 1985)
27. C. Heinecke, F.W. Hehl, Schwarzschild and Kerr solutions to Einstein's field equations: an introduction. Int. J. Mod. Phys. D (2015, in press)
28. W. Israel, Source of the Kerr metric. Phys. Rev. D **2**, 641–646 (1970)
29. G. Kaiser, Distributional sources for Newman's holomorphic Coulomb field. J. Phys. A **37**, 8735–8745 (2004)
30. S. Keppeler, *Spinning Particles—Semiclassics and Spectral Statistics* (Springer, Berlin, 2003)
31. M.K.-H. Kiessling, A.S. Tahvildar-Zadeh, A novel quantum-mechanical interpretation of the Dirac equation. eprint arXiv:1411.2296 (2014)

32. M.K.-H. Kiessling, A.S. Tahvildar-Zadeh, The Dirac point electron in zero-gravity Kerr–Newman spacetime. J. Math. Phys. **56**, 042303 (43) (2015)
33. T. Ledvinka, M. Žofka, J. Bičák, Relativistic disks as sources of Kerr–Newman fields, in *Proceedings of the 8th Marcel Grossmann meeting on general relativity, Jerusalem (1997)*, ed. by R. Ruffini (World Scientific, Singapore, 1998)
34. E.H. Lieb, M. Loss, *Analysis*, 2nd edn. (American Mathematical Society, Providence, 2010)
35. D. Lynden-Bell, Electromagnetic magic: the relativistically rotating disk. Phys. Rev. D **70**, 105017 (10) (2004)
36. G.C. McVittie, Dirac's equation in general relativity. Mon. Not. R. Astron. Soc. **92**, 868–877 (1932)
37. F. Melnyk, Wave operators for the massive charged linear Dirac field on the Reissner–Nordström metric. Class. Quantum Gravity **17**, 2281–2296 (2000)
38. E.T. Newman, E. Couch, K. Chinnapared, A. Exton, A. Prakash, R. Torrence, Metric of a rotating, charged mass. J. Math. Phys. **6**, 918–919 (1965)
39. D. Page, Dirac equation around a charged, rotating black hole. Phys. Rev. D **14**, 1509–1510 (1976)
40. A. Papapetrou, Rotverschiebung und Bewegungsgleichungen. Ann. Phys. **452**, 214–224 (1956)
41. C.L. Pekeris, The nucleus as a source in Kerr–Newman geometry. Phys. Rev. A **35**, 14–17 (1987)
42. E. Schrödinger, Diracsches Elektron im Schwerefeld. I. Sitzber. Preuss. Akad. Wiss. **11–12**, 105–128 (1932)
43. A. Sommerfeld, Über verzweigte Potentiale im Raum. Proc. Lond. Math. Soc. **s1-28**, 395–429 (1896)
44. E.C.G. Stückelberg, La mécanique du point matériel en théorie de relativité et en théorie des quanta. Helv. Phys. Acta **15**, 23–37 (1942)
45. K.G. Suffern, E.D. Fackerell, C.M. Cosgrove, Eigenvalues of the Chandrasekhar–Page angular functions. J. Math. Phys. **24**, 1350–1358 (1983)
46. A.S. Tahvildar-Zadeh, On the static spacetime of a single point charge. Rev. Math. Phys. **23**, 309–346 (2011)
47. A.S. Tahvildar-Zadeh, On a zero-gravity limit of the Kerr–Newman spacetime and its electromagnetic fields. J. Math. Phys. **56**, 042501 (19pp) (2015)
48. B. Thaller, Potential scattering of Dirac particles. J. Phys. A: Math. Gen. **14**, 3067–3083 (1981)
49. B. Thaller, *The Dirac Equation* (Springer, Berlin, 1992)
50. J. Weidmann, Absolut stetiges Spektrum bei Sturm-Liouville-Operatoren und Dirac-Systemen. Math. Z. **180**, 423–427 (1982)
51. M. Winklmeier, O. Yamada, Spectral analysis of radial Dirac operators in the Kerr-Newman metric and its applications to time-periodic solutions. J. Math. Phys. **47**, 102503 (17) (2006)
52. M. Winklmeier, O. Yamada, A spectral approach to the Dirac equation in the non-extreme Kerr–Newman metric. J. Phys. A **42**, 295204 (15) (2009)
53. A. Zecca, Dirac equation in Schwarzschild geometry. Nuovo Cim. B **113**, 1309–1315 (1998)
54. D.M. Zipoy, Topology of some spheroidal metrics. J. Math. Phys. **7**, 1137–1143 (1966)

Noncommutative Geometry and the Physics of the LHC Era

Christoph A. Stephan

Contents

Abstract Noncommutative geometry allows to unify the basic building blocks of particle physics, Yang-Mills-Higgs theory and general relativity, into a single geometrical framework. The resulting effective theory constrains the couplings of the standard model and reduces the number of degrees of freedom. After an introduction of the basic ideas of Noncommutative geometry, I will present its predictions for the standard model and the few known models beyond the standard model based on a classification scheme for finite spectral triples. Most of these models, including the Standard Model, are now ruled out by LHC data.

C.A. Stephan (✉)
Institut für Mathematik, Universität Potsdam, Am Neuen Palais 10, 14469 Potsdam, Germany
e-mail: stephan@math.uni-potsdam.de

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_20

But interesting extensions of the standard model which agree with the presumed Higgs mass, predict new particles (Fermions, Scalars and Bosons) and await further experimental data.

Keywords Noncommutative geometry • Beyond standard model • Spectral action

Mathematics Subject Classification (2010). Primary 99Z99; Secondary 00A00

1 Introduction

Noncommutative geometry as an algebraic approach to geometry has surprisingly proved to be a useful tool to understand the geometry of the standard model of particle physics. Connes' spectral triples allow to transfer geometrical notions from compact Riemannian spin manifolds to finite matrix spaces. The central object in this construction is a generalised Dirac operator which in such finite cases can be interpreted as a fermionic mass matrix of the particle model.

It came as a surprise that spectral triples, which were originally constructed to investigate for example singular foliations of manifolds, allow to incorporate the intricate structure of the standard model particle multiplets as well as its complicated representation theoretic structure. Product spaces built from spectral triples over manifolds and from finite spectral triples over matrix algebras proved to be very useful to construct models known from particle physics, in particular the standard model.

The Dirac operator is a central ingredient of a spectral triple and plays a multiple role. On the one hand it substitutes for the metric of the underlying space(-time), on the other hand it defines the dynamics of the fermions. If one constructs spectral triples for the standard model, the Higgs field becomes a natural part of the Dirac operator acting as an inter-twiner of representations. In the noncommutative context such scalar fields as the Higgs field are then interpreted as connections of the internal matrix space and are therefore considered as part of the metric.

In recent years the matrix geometries that underly the standard model have been classified in various ways. As another surprise it was found that the standard model not only fits into the noncommutative framework but is also in many ways a very minimal model and the chiral structure of the electro-weak sector appears to be quite natural in the setting of finite spectral triples.

But the classification schemes also allow to construct particle models beyond the standard model. These models generally have a rich phenomenology and may contribute interesting new insights to the dark matter problem which is probably one of the most important open question in today's particle physics.

These conference proceedings were written as a supplement to a talk given at conference *Quantum Mathematical Physics, A Bridge between Mathematics and*

Physics which took place in 2014 in Regensburg. The interested reader may profit from the talk and is referred to the web page [1].

The article is organised as follows. Section 2 aims to give an introduction into the notion of a spectral triple, its axioms, almost-commutative spectral triples which are central to the noncommutative approach to particle physics and some classification schemes for spectral triples. Furthermore it gives a short account of how gauge groups appear in the framework and how the relevant Dirac operators appear. In the third section we describe the spectral action which is a natural action functional on spectral triples. We also give an overview on alternative action functionals for Dirac operators. Some of those may naturally be applied in the Lorentzian setting. The fourth section deals with the predictions noncommutative geometry makes for the standard model and its short-comings in the light of recent experimental data, in particular the detection of a Higgs-like boson by the LHC experiments. The fifth section gives examples of models beyond the standard model with a particular focus on an extension which displays new fermions, gauge bosons and a new scalar field. This model seems to agree with experimental data and may provide interesting dark matter candidates. We end this article with some questions to noncommutative geometry and particle physics.

2 Spectral Triples

We try to give a short introduction into the basic concepts of noncommutative geometry as needed for particle physics. For more in-depth introductions we recommend the classical book of Connes [2] and the more recent general overview of Connes and Marcolli [3].

For a pedagogical introduction to spectral triples we recommend Khalkhali's textbook [4] and for details on the particle physics side of the subject the excellent book by van Suijlekom [5] and the lecture notes of Schücker [6].

2.1 General Definitions

Let us give a brief account on the basic ingredients of noncommutative geometry in the formulation given by Connes [2, 7]. The basic geometric building blocks are *spectral triples* $(\mathcal{A}, \mathcal{D}, \mathcal{H})$ which, in the even, real case, are given by the following five components:

- a unital pre-C^* algebra $\mathcal{A}$.
- a separable Hilbert space $\mathcal{H}$ on which the algebra is faithfully represented with the representation $\rho : \mathcal{A} \to End(\mathcal{H})$.
- an unbounded self-adjoint operator $\mathcal{D} : dom(\mathcal{D}) \to \mathcal{H}$ with compact resolvent. This operator will be referred to as the *Dirac operator*.

- an anti-unitary operator $J : \mathcal{H} \to \mathcal{H}$. In the mathematical literature J is referred to as the *real structure* while in physics literature it is usually called the *charge conjugation operator*.
- a unitary operator $\gamma : \mathcal{H} \to \mathcal{H}$, the abstract *volume element* or *chirality operator*.

Example The standard example of a spectral triple is build on a compact n-dimensional Riemannian spin-manifold (M, g). In this case the algebra $\mathcal{A} = C^\infty(M)$ and the Hilbert space consists of the square-integrable spinors $\mathcal{H} = L^2(\Gamma(\Sigma))$. The representation of the algebra on the Spinors is simply by pointwise multiplication. The Dirac operator is the standard Dirac operator associated to the Levi-Civita connection ∇ and is locally given by $(\not{\partial}\psi)(x) := \sum_i e_i \cdot \nabla_{e_i}\psi(x)$, where e_i, $i = 1, .., n$ form an orthonormal basis of the tangent space $T_x(M)$ and $X\cdot$ denotes the Clifford multiplication of a vector. The charge conjugation and the volume element are the standard operators from particle physics.

The five components of the spectral triple are required to fulfil the following set of axioms in order to constitute a spectral triple:

Axiom 1 This axiom assumes that there exists a classical (spectral) dimension n associated to the growth of the eigenvalues of the Dirac operator. It is also referred to as the axiom of finite summability. Since the resolvent of $\mathcal{D}$ is compact its eigenvalues form a decreasing sequence $\{\alpha_i\}$. The axiom then states that there is a smallest $n \in \mathbb{N}$ such that the ith eigenvalue is asymptotically for $i \to \infty$ of the order of $\mathcal{O}(i^{-1/n})$. This smallest n is defined as the *dimension* of the spectral triple.

Remark 2.1 The dimension of a spectral triple can be zero. Indeed this happens for finite spectral triples build from matrix algebras which play a central rôle in noncommutative approach to particle physics.

Remark 2.2 The dimension of the spectral triple of an n-dimensional Riemannian spin manifold coincides by Weyl's law for the growth of eigenvalues of $\not{\partial}$ with the dimension of the manifold.

Axiom 2 This axiom requires that the commutator of the Hilbert space representation of each element in the algebra with the Dirac operator is a bounded operator on $\mathcal{H}$. So we have for all $a \in \mathcal{A}$ that $[\mathcal{D}, \rho(a)] \in \mathcal{B}(\mathcal{H})$.

From now on we will drop the explicit mentioning of the representation ρ when no confusion arises.

Remark 2.3 This axiom certainly holds for the spectral triple of a manifold since the commutator of the Dirac operator with a differentiable function equals Clifford multiplication with its differential, i.e. $[\not{\partial}, f]\psi = df^\sharp \cdot \psi, f \in C^\infty(M)$ and $\psi \in \Gamma(\Sigma)$.

Axiom 3 The Dirac operator is a first-order operator. In the algebraic setting of spectral triples the axiom states that for all $a, b \in \mathcal{A}$ we have $[[\mathcal{D}, a], JbJ^{-1}] = 0$.

Remark 2.4 This axiom can again be checked easily for the spectral triple of a manifold since $[\not{\partial}, f]$ is a zero-order differential operator for all $f \in C^\infty(M)$ and therefore commutes with any function in the algebra.

Axiom 4 The axiom of strong regularity states that the elements of the algebra are differentiable in a suitable way. For any bounded operator $T \in \mathcal{B}(\mathcal{H})$ we define define $\delta(T) := [|\mathcal{D}|, T]$ where $dom\,\delta = \{T \in \mathcal{B}(\mathcal{H}) | T(dom|\mathcal{D}|) \subset (dom|\mathcal{D}|)$ and $\delta(T) \in \mathcal{B}(\mathcal{H})\}$. Furthermore we define $\mathcal{H}^\infty := \bigcap_{j=1}^{\infty} dom\,\mathcal{D}^j$.

The axiom demands that $\mathcal{A}$, $[\mathcal{D}, \mathcal{A}]$ and $End_{\mathcal{A}}(\mathcal{H}^\infty)$ are in

$$B^\infty(\mathcal{H}) := \bigcap_{j=1}^{\infty} dom \circ^j.$$

Axiom 5 The orientability axiom gives further conditions on the chirality operator. It demands that $\gamma^2 = id_{\mathcal{H}}$ and if the dimension n of the spectral triple is even that $\gamma\mathcal{D} = -\mathcal{D}\gamma$. In the odd-dimensional case $\gamma = id_{\mathcal{H}}$. Furthermore we require that γ can be represented by a Hochschild n-cycle. For further details of this axiom we refer to [7].

Remark 2.5 For the spectral triple of a manifold the abstract volume form γ coincides with the Clifford multiplication of the metric volume form $dvol_g$.

Axiom 6 The reality axiom demands a set of commutation relations for the real structure J with the other operators. In particular we have $J^2 = \epsilon$, $J\mathcal{D} = \epsilon'\mathcal{D}J$ and $J\gamma = \epsilon''\gamma J$ where the signs are given in the following table.

p mod 8	0	1	2	3	4	5	6	7
ϵ	+	+	−	−	−	−	+	+
ϵ'	+	+	+	+	+	−	+	+
ϵ''	+	−	−	+	+	+	−	+

Here the p is the so called *KO*-dimension. We require also that $[JaJ^{-1}, b] = 0$ for all $a, b \in \mathcal{A}$, i.e. that JaJ^{-1} is in the opposite algebra $\mathcal{A}^{op}$.

For the spectral triple of a manifold the *KO*-dimension is usually taken to be equal to the dimension of the manifold itself. In the finite case of matrix algebras this requirement is dropped and it is precisely the fact that the *KO*-dimension and the dimension of the spectral triple need not coincide that allows Majorana mass terms for neutrinos.

That the abstract definition of a spectral triple gives for commutative $\mathcal{A}$ an equivalent definition for a compact Riemannian spin manifold is the central content of *Connes' reconstruction theorem*. See Connes [7, 8] for an in depth proof of the theorem and Sanders [9] for a very readable introduction.

Note that the definition of a spectral triple does not require that the algebra $\mathcal{A}$ is commutative. It is precisely this possibility to pass to noncommutative algebras which allows to generalise the frame work to *noncommutative spaces*.

Example To give an example of how to reconstruct geometric data from a spectral triple let us consider the spectral triple of a manifold

$$(C^\infty(M), L^2(\Gamma(\Sigma)), \not{\partial}).$$

As we have mentioned above, the dimension of the manifold M can be recovered by Weyl's law from the growth of the eigenvalues of $\not{\partial}$. The metric distance $d(p,q)$, $p,q \in M$, can be reconstructed from Connes' distance formula $d(p,q) := \sup_{f \in C^\infty(M)} (|\delta_p(f) - \delta_q(f)| : ||[\not{\partial}, f]|| \leq 1||$ where $\delta_p(f) = f(p)$ are δ-distributions. This formula can be generalised to any spectral triple if we replace the δ-distributions by states on the algebra.

Remark 2.6 Suppose we are given the algebra $\mathcal{A}$, the Hilbert space $\mathcal{H}$, the representation of the algebra ρ, the real structure J and the chirality operator γ. Then these data in generally do not uniquely fix the Dirac operator $\mathcal{D}$. In the case of the spectral triple over a Riemannian manifold (M, g) one may for example replace the Dirac operator associated to the Levi-Civita connection by a Dirac operator associated to any connection compatible with the metric g, i.e. by a connection with torsion [10]. One can also add scalar potentials [11] or terms of higher form degrees, as long as they are compatible with the axioms. Here we will always assume that the Dirac operator is associated to the Levi-Civita connection.

Definition 2.7 Given all the components $(\mathcal{A}, \mathcal{H}, \rho, J, \gamma)$ of a real, even spectral triple save the Dirac operator. Then the configuration space of Dirac operators $\mathcal{C}(\mathcal{A})$ is defined to be

$$\mathcal{C}(\mathcal{A}) := \{\mathcal{D} : dom(\mathcal{D}) \subset \mathcal{H} \to \mathcal{H} | (\mathcal{A}, \mathcal{H}, \mathcal{D}) \text{ is a real, even, spectral triple}\}$$

The configuration space $\mathcal{C}(\mathcal{A})$ is in general too big for applications in physics. So one will usually choose a sub-space which has certain invariance or covariance properties. In the case of particle physics models this will in general be the space of generalised Dirac operator which can be interpreted as twisted Dirac operators associated to suitable principal fibre bundles.

It should be noted that spectral triples are tailored to describe Riemannian manifolds. But it is quite clear that to model physical space-time one would need a Lorentzian equivalent for a spectral triple. The endeavour to find a suitable replacement in the Lorentzian case proves to be an extremely difficult task. Some proposals have been made by Strohmaier [12], Paschke and Sitarz [13], Besnard [14], Franco and Eckstein [15] and others. But no conclusive definition has been achieved, yet. It seems that a major obstacle in the definition is the fact, that on a Lorentz manifold the Dirac equation has no solutions in a suitable Hilbert space. Solutions spaces of wave operators consist generally of tempered distributions and are therefore not square integrable.

2.2 Almost-Commutative Geometries

Spectral triples have the nice property that the tensor product of two spectral triples is again a spectral triple. This also holds for the even, real case with real structure and chirality operator discussed above. Given two spectral triples $(\mathcal{A}_1, \mathcal{D}_1, \mathcal{H}_1, J_1, \gamma_1)$ and $(\mathcal{A}_2, \mathcal{D}_2, \mathcal{H}_2, J_2, \gamma_2)$ one constructs a new spectral triple $(\mathcal{A}, \mathcal{D}, \mathcal{H}, J, \gamma)$ with the data

- $\mathcal{A} := \mathcal{A}_1 \otimes \mathcal{A}_2$
- $\mathcal{H} := \mathcal{H}_1 \otimes \mathcal{H}_2$
- $J := J_1 \otimes J_2$
- $\gamma := \gamma_1 \otimes \gamma_2$
- $\mathcal{D} := \mathcal{D}_1 \otimes id_{\mathcal{H}_2} + \gamma_1 \otimes \mathcal{D}_2$

If we want to construct particle models from spectral triples it turns out that such products are very useful. In reminiscence to Kaluza-Klein theory one takes the spectral triple of a compact Riemannian spin manifold and tensorises with a finite spectral triple. A finite spectral triple is defined as follows.

Definition 2.8 A *finite spectral triple* is given by a matrix algebra with m summands $A_f := \bigoplus_{j=1}^{m} \mathrm{Mat}_j(n_j, \mathbb{K}_j)$, where $n_j \in \mathbb{N}$, $\mathbb{K}_j = \mathbb{R}, \mathbb{C}, \mathbb{H}$, a finite Hilbert space $H_f := \mathbb{C}^N$ and a Dirac operator $D_f \in \mathrm{Mat}(N, \mathbb{C})$ such that (A_f, H_f, D_f) with suitable real structure J_f and γ_f constitute a zero-dimensional spectral triple of *KO*-dimension p.

One of the reasons why such finite spectral triples are useful in particle physics is the fact that the group of unitaries $U(A_f) := \{u \in A_f | u^* u = uu^* = id\}$ of the matrix algebra can be identified, when properly lifted to the automorphisms of the Hilbert space, with the structure group underlying the particle model. One can then interpret the tensor product of the L^2-spinors and the finite Hilbert space as a twisted spinor bundle associated to the fibre bundle product of the spin structure and a trivial vector bundle associated to a (trivial) principle fibre bundle associated to said structure group. There are at the moment two approaches to define the structure group of the particle model and we will come back to this point later.

In the context of particle physics the Hilbert space is the finite Hilbert space of particle multiplets. In this case its rank N is even and one has to count particles and anti-particles as well as left-handed and right-handed particles separately. Consequently the Hilbert space is four times too big and the construction of the Dirac action requires a projection on the physical Hilbert space. The Dirac operator plays the rôle of the fermionic mass matrix and encodes the Yukawa couplings as well as possible Dirac or Majorana mass terms. The real structure is then indeed the charge conjugation operator from particle physics and the volume form can be identified with the chirality operator that allows to project on left- and right-handed spinors. It turns out that the *KO*-dimension should be chosen to $p = 6$ so we will only consider this case. This choice of *KO*-dimension allows for Majorana masses for right-handed neutrinos in the standard model, Barrett [16] as well as

Chamseddine, Connes and Marcolli [17]. But such Majorana masses are in conflict with the axiom of orientability [18]. *KO*-dimension six also implies that the number of summands in the matrix algebra A_f has to be even.

Definition 2.9 Given the spectral triple of a 4-dimensional Riemannian spin manifold and a finite spectral triple, we call their tensor product an *almost-commutative spectral triple*.

Example The standard example of such an almost-commutative geometry is the spectral triple of the standard model. We will give the finite matrix algebra, its representation on the Hilbert space and the Dirac operator in some detail to illustrate the general structure of particle models in terms of spectral triples.
The finite algebra can be chosen to be

$$A_f = \mathbb{C} \oplus \mathbb{H} \oplus M(3,\mathbb{C}) \oplus \mathbb{C}.$$

We see that the group of unitaries is $U(A_f) = U(1) \times SU(2) \times U(3) \times U(1)$. The correct way to deal with the supplementary $U(1)$ terms to obtain the standard model structure group $G_{SM} = U(1) \times SU(2) \times SU(3)$ will be explained later. The finite Hilbert space is taken from particle physics. It splits into four subspaces $H_f := H_L \oplus H_R \oplus H_L^c \oplus H_R^c = \mathbb{C}^{96}$ which are given by

$$H_L = (\mathbb{C}^2 \otimes \mathbb{C}^3 \otimes \mathbb{C}) \oplus (\mathbb{C}^2 \otimes \mathbb{C}^3 \mathbb{C}^3)$$

and

$$H_R = (\mathbb{C} \otimes \mathbb{C}^3 \otimes \mathbb{C}) \oplus (\mathbb{C} \otimes \mathbb{C}^3 \otimes \mathbb{C}) \oplus (\mathbb{C} \otimes \mathbb{C}^3 \otimes \mathbb{C}^3) \oplus (\mathbb{C} \otimes \mathbb{C}^3 \otimes \mathbb{C}^3),$$

where the superscript $\cdot^c$ denotes the anti-particle spaces. One can choose as a basis for the Hilbert space the particle multiplets of the standard model, i.e.

$$\begin{pmatrix} e \\ \nu_e \end{pmatrix}_L, \begin{pmatrix} \mu \\ \nu_\mu \end{pmatrix}_L, \begin{pmatrix} \tau \\ \nu_\tau \end{pmatrix}_L, \begin{pmatrix} u \\ d \end{pmatrix}_L, \begin{pmatrix} c \\ s \end{pmatrix}_L, \begin{pmatrix} t \\ b \end{pmatrix}_L,$$

for the left-handed $SU(2)$-doublets and

$$e_R,\ \nu_{eR},\ \mu_R,\ \nu_{\mu R},\ \tau_R,\ \nu_{\tau R},\ u_R,\ d_R,\ c_R,\ s_R,\ t_R,\ b_R$$

for the right-handed $SU(2)$-singlets.

Furthermore we have the following representation ρ of algebra elements

$$(a,b,c,d) \in \mathcal{A}_f = \mathbb{C} \oplus \mathbb{H} \oplus M_3(\mathbb{C}) \oplus \mathbb{C}$$

which also decomposes into for direct summands $\rho = \rho_L \oplus \rho_R \oplus \rho_L^c \oplus \rho_R^c$ that are given by

$$\rho_L(a,b,c,d) = \begin{pmatrix} b \otimes 1_3 \otimes 1_3 & 0 \\ 0 & b \otimes 1_3 \end{pmatrix},$$

$$\rho_R(a,b,c,d) = \begin{pmatrix} a1_3 \otimes 1_3 & 0 & 0 & 0 \\ 0 & \bar{a}1_3 \otimes 1_3 & 0 & 0 \\ 0 & 0 & \bar{d}1_3 & 0 \\ 0 & 0 & 0 & \bar{a}1_3 \end{pmatrix},$$

$$\rho_L^c(a,b,c,d) = \begin{pmatrix} 1_2 \otimes 1_3 \otimes c & 0 \\ 0 & d \otimes 1_3 \otimes 1_2 \end{pmatrix}$$

and

$$\rho_R^c(a,b,c,d) = \begin{pmatrix} 1_3 \otimes c & 0 & 0 & 0 \\ 0 & 1_3 \otimes c & 0 & 0 \\ 0 & 0 & d1_3 & 0 \\ 0 & 0 & 0 & d1_3 \end{pmatrix}.$$

The real structure is

$$J_f = \begin{pmatrix} 0 & 1_{48} \\ 1_{48} & 0 \end{pmatrix} \circ \text{complex conjucation}$$

and the chirality operator is the diagonal matrix $\gamma_f = \text{diag}(-1_{24}, 1_{24}, 1_{24}, -1_{24})$. Note that the signs discriminating left-handed and right-handed particles change from the particle sector to the anti-particle sector. This is due to the fact that we construct a spectral triple of *KO*-dimension six.

A central object in the whole construction is the Dirac operator D_f. It maps left-handed particles to right-handed particles and vice versa but also contains Majorana mass terms which map right-handed neutrinos to right-handed anti-neutrinos. Therefore the configuration space of Dirac operators consists of matrices $D_f \in \mathcal{C}(A_f) \subset Mat(96, \mathbb{C})$ that split into four blocks

$$D_f = \begin{pmatrix} \Delta & H \\ H^* & \bar{\Delta} \end{pmatrix}$$

where each block is a matrix, i.e. $\Delta, H \in Mat(48, \mathbb{C})$. The Dirac operator is selfadjoint with respect to the standard inner product on $H_f = \mathbb{C}^{96}$ and its block Δ decomposes into the following sub-matrices

$$\Delta = \begin{pmatrix} 0 & M \\ M^* & 0 \end{pmatrix}$$

with

$$M = \left(\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes M_e + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes M_\nu \right)$$

$$\oplus \left(\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes M_u \otimes 1_3 + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes M_d \otimes 1_3 \right).$$

Here we have the lepton mass matrices $M_e = \mathrm{diag}(m_e, m_\mu, m_\tau)$ and $M_\nu = C_{PMNS}\,\mathrm{diag}(m_{\nu_e}, m_{\nu_\mu}, m_{\nu_\tau})$ with the unitary PMNS-mixing matrix for the neutrinos as well as the quark mass matrices $M_u = \mathrm{diag}(m_u, m_c, m_t)$ and $M_d = C_{CKM}\,\mathrm{diag}(m_d, m_s, m_b)$ with the unitary CKM-mixing matrix. Since the Majorana mass matrix H contains mainly entries equal to zero, apart from a 3×3 sub-matrix for the Majorana masses of the right-handed neutrinos, we will not give the details and refer to [17].

The final spectral triple of the standard model is then the tensor product of the finite spectral triple given above and the commutative spectral triple of a 4-dimensional compact Riemannian spin manifold $(C^\infty(M), L^2(\Gamma(\Sigma)), \not{\partial})$. The almost commutative algebra $C^\infty(M) \otimes A_f$ can be seen as the algebra of smooth functions on M with values in the matrix algebra A_f. We notice that the (lifted) unitary group of $C^\infty(M) \otimes A_f$ is coordinate-dependent and therefore it can be identified with the gauge group of a (trivial) principal fibre bundle.

2.3 Classifications of Finite Spectral Triples

In consideration of the complexity of the standard model's finite spectral triple one could (and should) ask the question how unique or at least how special this model is under certain extra assumptions. It therefore appears worthwhile to classify all possible finite spectral triples and, if the general classification turns out to yield too many spectral triples, find suitable conditions to single out spectral triple of interest to particle physics.

A complete and general classification has been performed independently by Paschke and Sitarz [19] and by Krajewski [20]. Although the possible particle models that can be built from finite geometries are strictly less than the models which can be constructed in the classical formalism based on fibre bundles, it is nevertheless a far too big set. We will briefly comment here on two proposals to cut down this set of all finite spectral triples to sub-sets of potential physical interest.

Let us first mention a recent classification scheme proposed by Connes and Chamseddine [21]. In this approach extra mathematical conditions are imposed on the finite algebra and its representation. One assumes that the action of the algebra has a separating vector and that the representation, i.e. the Hilbert space

is irreducible. The second conditions demands that there are no nontrivial linear projections acting on the Hilbert space which commute with the representation of the algebra and the action of the real structure.

Applying these conditions to a finite matrix algebra one is essentially left with two summands over the complex numbers, i.e. $A_f = Mat(k, \mathbb{C}) \oplus Mat(k, \mathbb{C})$. If one imposes as a further condition that the algebra should be symmetric under a certain symplectic symmetry, one finds that only algebras of the type $A_f = Mat(r, \mathbb{H}) \oplus Mat(k, \mathbb{C})$ are allowed. The commutation relations with the chirality operator then require that r is an even number and the first realistic model turns out to have the algebra $A_{PS} = \mathbb{H} \oplus \mathbb{H} \oplus Mat(4, \mathbb{C})$.

We note that A_{PS} has a three-summand version of the standard model algebra as a sub-algebra, namely $\mathbb{C} \oplus \mathbb{H} \oplus Mat(3, \mathbb{C}) \subset \mathbb{H} \oplus \mathbb{H} \oplus Mat(4, \mathbb{C})$. It was shown by Connes, Chamseddine and van Suijlekom [22] that the particle model of the corresponding spectral triple is the well known Pati-Salam model.

An earlier classification scheme was proposed by Iochum, Jureit, Schücker and Stephan [23]. Here the idea was to put up a list of restrictions on the resulting particle models, that appear necessary from the point of view of particle physics. The models obtained from this classification proved to be very useful for a bottom-up approach in model building which has been exploited in [24, 25] and for the model [26] which will be discussed in more detail below.

The requirements are such that the resulting particle model should

- be irreducible i.e. to have the smallest possible internal Hilbert space (minimal approach),
- allow a non-degenerate Fermionic mass spectrum,
- be free of harmful gauge anomalies,
- have unbroken colour groups
- and possess no charged massless Fermions.

Carrying out the classification is a demanding combinatorial task [27] and has been done for up to six summands in the matrix algebra A_f [23] and can be summarised as follows in terms of A_f:

♯ summands	A_f
2	No model
4	$\mathbb{C} \oplus Mat(2, \mathbb{C}) \oplus Mat(n, \mathbb{K}) \oplus \mathbb{C}$ $\mathbb{C} \oplus \mathbb{C} \oplus \mathbb{C} \oplus Mat(n, \mathbb{K})$
6	$\mathbb{C} \oplus Mat(2, \mathbb{C}) \oplus Mat(n_1, \mathbb{K}_1) \oplus \mathbb{C} \oplus \mathbb{C} \oplus Mat(n_2, \mathbb{K}_2)$ $\mathbb{C} \oplus \mathbb{C} \oplus \mathbb{C} \oplus Mat(n_1, \mathbb{K}_1) \oplus \mathbb{C} \oplus \mathbb{C} \oplus \mathbb{C} \oplus Mat(n_2, \mathbb{K}_2)$

We call spectral triples with the matrix algebra $A_f = \mathbb{C} \oplus Mat(2, \mathbb{C}) \oplus Mat(n, \mathbb{K}) \oplus \mathbb{C}$ of standard model type. The sub-algebra $Mat(n, \mathbb{K})$ is called the colour algebra. The corresponding Hilbert space, representation of the algebra, real structure, chirality operator and configuration space of Dirac operators coincide in their

general form with those of the standard model, thus the denomination. Note that in this classification scheme neither the number n of colours nor the field $\mathbb{K}$ can be determined. They rest as an input from experiment. Spectral triples with matrix algebra $A_f = \mathbb{C} \oplus \mathbb{C} \oplus \mathbb{C} \oplus Mat(n, \mathbb{K})$ are called of electro-strong type since the sub-algebra $Mat(n, \mathbb{K})$ is a colour algebra.

From the classification follows that the standard model is indeed one of the simpler models within the set of spectral triples. Furthermore the two types of spectral triples we found from the classification turned out to be very useful basic building blocks to construct models beyond the standard model.

2.4 Gauge Groups

Up to now we have defined spectral triples with their configuration spaces of Dirac operators and have classified certain interesting subsets. But the configuration spaces of Dirac operators is still far too big and we wish to constrain them by specifying a gauge or structure group. The Hilbert space can be considered as a space of sections of a vector (spinor) bundle associated to a principal fibre bundle. We will now define the necessary structure group for finite spectral triples with an almost-commutative spectral triple.

Following Lazzarini and Schücker [28] we define the unitary automorphism group of the Hilbert space of a spectral triple. It is a sub-group of the general automorphism group of the Hilbert space and contains those unitary automorphisms that are compatible with the structures of the spectral triple.

Definition 2.10 Let $(\mathcal{A}, \mathcal{H}, \mathcal{D})$ be a real, even spectral triple with real structure J and chirality operator γ. The automorphism group of the Hilbert space is defined as

$$Aut_{\mathcal{A}}(\mathcal{H}) := \{U \in End(\mathcal{H}) | UU^* = U^*U = id_{\mathcal{H}},\ UJ = JU,$$
$$U\gamma = \gamma U,\ U\rho(\mathcal{A})U^{-1} \subset \rho(\mathcal{A})\}$$

where ρ is the representation of the algebra on the Hilbert space.

The last condition is called *covariance condition*. It ensures for example, that the leptons and the quarks are charged under the same weak $SU(2)$-sub-group in the case of the standard model.

Example For the standard model spectral triple one finds the following automorphism group of the Hilbert space [28]

$$Aut_{A_f}(H_f) = [U(2)_w \times U(3)_c \times \prod_{j=1}^{6} U(3)]/[U(1) \times U(1)]$$

We notice that this group is larger than the standard model structure group $U(1) \times SU(2) \times SU(3)$. It contains family mixing unitaries $\prod_{j=1}^{6} U(3)$ and can therefore only be considered as a receptacle group for the true structure group.

In almost-commutative geometry the true structure group is identified with the group of unitaries of the algebra lifted to the Hilbert space or with a certain subgroup which is then centrally extended. Let us first give the definition of a structure group following Connes and Chamseddine [29]. Assume that $u \in U(A_f)$. The lift of u to the automorphisms of the finite Hilbert space is then defined by

$$L(u) := \rho(u) J \rho(u) J^{-1}.$$

The structure group of the principal fibre bundle is then $G^{cc} := \{L(u) | u \in U(A_f), \det(u) = 1\}$. The last condition is called the unimodularity condition. So one can consider now the Hilbert space of the almost-commutative spectral triple as the space of sections associated to the principal fibre bundle $P = P_{Spin} \circ P_{G^{cc}}$ where P_{Spin} is the natural spin structure.

A second approach that eliminates the need of the unimodularity condition was developed by Lazzarini and Schücker [28]. It restricts the unitaries which are to be lifted to the non-commutative unitaries $U^n(A_f)$, i.e. the unitaries of the non-abelian matrix summands in the finite algebra. Here one apparently loses all the $U(1)$-sub-groups which play an important part in the standard model. Yet, they can be reintroduced by centrally extending the lift w.r.t. the determinant of the the non-commutative unitaries. Let us denote this lift by $\mathbb{L} : U^n(A_f) \to Aut_{A_f}(H_f)$ without giving the details (they are quite technical and we refer the interested reader to [28]). But we note that the lift is not unique. In particular the central charges of the central extension can be chosen freely. They are usually fixed on physical grounds by demanding that the resulting particle model be free of harmful $U(1)$-anomalies.

Definition 2.11 The structure group is in this case $G_f := \{\mathbb{L}(u) | u \in U^n(A_f)\}$ with chosen central extension for the lift $\mathbb{L}$.

In the extensions of the standard model we will usually work with this definition as it proves to be more flexible than the original one by Chamseddine and Connes.

We notice that the almost-commutative Dirac operator $\not{\partial} \otimes 1 + dvol \cdot \otimes D_f$ is not gauge covariant and therefore not a Dirac operator induced by the associated principal fibre bundle $P = P_{Spin} \circ P_{G_f}$. So one defines the *fluctuated Dirac operator* $\mathcal{D}^f$. The finite Dirac operator D_f gets promoted to an inter-twiner $\Phi(D_f) \in End(L^2(\Gamma(\Sigma)) \otimes H_f)$ adapted to the principal fibre bundle P_{G_f}. We will always assume that the fields that constitute the inter-twiner are minimal in the sense that for two sub-groups of G_f we only have one scalar multiplet of inter-twiners. This assumption avoids the possibility of different Higgs fields for leptons and quarks. We will also assume that the scalar fields that constitute the inter-twiner allow to recover the finite Dirac operator if replaced by the identity, i.e. $\Phi(D_f) \to D_f$.

The derivative part $\not{\partial} \otimes 1$ gets promoted to a twisted Dirac operator $\not{\partial} \otimes 1 + \sum_j e_j \cdot \nabla_j^f$ where ∇^f is a covariant derivative associated to P_{G_f}. One can define algorithms

to obtain such fluctuated Dirac operators operationally and we refer to Connes and Chamseddine [29] for details.

Definition 2.12 For a given almost commutative spectral triple we define the set of covariant Dirac operators to be

$$\mathcal{C}^{cov}(\mathcal{A}) := \{\mathcal{D}^f = \not{\partial} \otimes 1 + \sum_j e_j \cdot \nabla_j^f + dvol \cdot \Phi(D_f)\}.$$

This will be the final dynamical configuration space of Dirac operators for the particle model. Note that the covariant Dirac operators form a subset of the configuration space of Dirac operators of the almost-commutative spectral triple.

3 Action Principles

One of the central objects in the noncommutative approach to the standard model is the (covariant) almost-commutative Dirac operators. Therefore Chamseddine and Connes proposed an action principle on the space of Dirac operators called *spectral action*. This action has the disadvantage that it needs a Dirac operator with discrete eigenvalues and is therefore only well defined on compact Riemannian manifolds. We will discuss this point briefly when we consider alternative approaches to define an action for Dirac operators.

3.1 The Spectral Action

The Chamseddine-Connes spectral action [29] for a spectral triple is defined to be the number of eigenvalues of the $\mathcal{D}$ in an interval $[-\Lambda, \Lambda]$ where Λ is a positive real number. One usually considers the spectral action to be an effective action for the gauge bosons which is valid at Λ and subject to renormalisation when one wishes to investigate different energy scales. For the fermions the action is given by the Dirac action for $\mathcal{D}$ with a projection on the physical Hilbert space.

Since it is not possible to calculate the spectral action exactly from the above definition, one smoothes the counting function and resorts to an alternative definition which allows for approximate calculations. We take this approximation as the actual definition of the spectral action.

Definition 3.1 Let f be a smooth cut-off function with support in $[0, +1]$ which is constant near zero and let $\Lambda \in \mathbb{R}^+$. The bosonic spectral action for the Dirac operator $\mathcal{D}$ is

$$S_{cc}(\mathcal{D}) := \mathrm{Tr} f\left(\frac{\mathcal{D}^2}{\Lambda^2}\right).$$

The trace Tr is the trace over the Hilbert space.

Performing a Laplace transform one gets from the heat trace asymptotics for $t \to 0$

$$\mathrm{Tr}\left(e^{-t\,\mathcal{D}^2}\right) \sim \sum_{n\geq 0} t^{n-2} a_{2n}(\mathcal{D}^2)$$

with Seeley-deWitt coefficients $a_{2n}(\mathcal{D}^2)$. For the spectral action S_{cc} follows (by $t = \Lambda^{-2}$) an asymptotic expansion

$$S_{cc}(\mathcal{D}) \sim \Lambda^4 f_4\, a_0(\mathcal{D}^2) + \Lambda^2 f_2\, a_2(\mathcal{D}^2) + \Lambda^0 f_0\, a_4(\mathcal{D}^2) + O(\Lambda^{-\infty})$$

as $\Lambda \to \infty$ with f_4, f_2, f_0 moments of cut-off function f.

Assume from now on that D is the covariant Dirac operator of an almost-commutative spectral triple, i.e. it is of the form $D = \partial\!\!\!/ \otimes 1 + \sum_j e_j \cdot \nabla_j^f + dvol \cdot \Phi(D_f)$. Assume further that the underlying manifold M is closed and $\dim(M) = 4$.

The calculations of the Seeley-DeWitt coefficients are long but standard. So we give here the final results in a condensed notation. The a_0-coefficient is essentially the volume of the manifold and will not concern us here. So we focus on the a_2- and the a_4-coefficient:

$$\begin{aligned}
a_2(D) &= -\tfrac{dim(H_f)}{96\pi^2} \int_M R\, dvol - \tfrac{1}{48\pi^2} \int_M tr(\Phi^2) dvol \\
a_4(D^2) &= \tfrac{11\, dim(H_f)}{720}\, \chi(M) - \tfrac{dim(H_f)}{320\pi^2} \int_M \|W\|^2\, dvol \\
&\quad + \tfrac{1}{8\pi^2} \int_M tr\big([\nabla^{\mathcal{H}_f}, \Phi]\big) + tr(\Phi^4) dvol \\
&\quad + \tfrac{5}{96\pi^2} \int_M tr\big(\Omega_f^2\big) dvol + \tfrac{1}{48\pi^2} \int_M R\, tr(\Phi^2) dvol
\end{aligned}$$

where R is the scalar curvature of M, $\chi(M)$ is the Euler characteristic, W is the Weyl tensor of M and $tr(\Omega_f^2)$ is the Yang-Mills Lagrangian of the covariant derivative ∇^f. We notice that the two terms

$$-\tfrac{1}{48\pi^2} \int_M tr(\Phi^2) dvol$$

and

$$+\tfrac{1}{8\pi^2} \int_M tr\big([\nabla^{\mathcal{H}_f}, \Phi]\big) + tr(\Phi^4) dvol$$

provide us exactly with the Lagrangian of a scalar field that can act as a Higgs field. In particular they exhibit the "Mexican hat"-potential which can induce a symmetry breaking mechanism.

Note also that the quartic term for the scalar potentials as well as the Yang-Mills Lagrangian for the covariant derivative appear in the same Seeley-DeWitt coefficient a_4. If we decompose into the Yang-Mills Lagrangians of the sub-groups of the finite structure group G_f and write it out in terms of the gauge coupling constants we obtain relations among the quartic couplings of the scalar fields in the inter-twiner $\Phi(D)$ and the gauge couplings [29]. These relations are not stable under renormalisation group flow and are therefore considered as boundary conditions for the flow, i.e. the spectral action is an effective action valid at the cut-off energy Λ. We notice furthermore that the trace of the square and the fourth power of the finite Dirac operator D_f also enter the relations among the quartic couplings and the gauge couplings. In this way also the Yukawa couplings get involved.

Further restrictions on the Yukawa couplings can be obtained by normalising the scalar fields to their proper mass dimension. In the present normalisation the fields have mass dimension 2. It was discovered by Tolksdorf and Thumstädter [30] that a proper normalisation of the bosonic and the fermionic action results in a new constraint on the trace of D_f^2, i.e. on the trace of the squared Yukawa matrix.

These constraints can be exploited to make the resulting particle models more predictive than the usual models based on the differential geometric Yang-Mills-Higgs approach. They provide extra boundary conditions at the cut-off energy which have to match the measured values at other energies via renormalisation group running.

3.2 Alternative Action Principles

Let give us give a short account on alternative approaches to action principles based on a Dirac operator. The first one is closely related to the spectral action. It is basically another way to regularise the counting function for the eigenvalues.

Kurkov, Lizzi, Sakellariadou and Watcharangkool [31] recently proposed to use a ζ-function regularisation to give a well defined value to the counting function of the eigenvalues. The value of the ζ-regularised spectral action can be given in terms of Seeley-DeWitt coefficients and turns out to be proportional to the a_4-coefficient. This way of regularising the counting function is closely related to the definition of the spectral action as Weyl anomaly as suggested by Andrianov, Kurkov and Lizzi [32]. As the spectral action of Chamseddine and Connes this approach is only well defined on compact Riemannian manifolds. It was noted by Zahn [33] that the Weyl anomaly, if calculated on a globally hyperbolic Lorentzian manifold, leads to similar results and may serve as a Lorentzian substitute.

A second approach which builds on a wider class of Dirac operators was developed by Tolksdorf [34, 35]. Here the generalised Dirac operators contain also curvature terms of the gauge connection as well as higher powers of the inter-twiner scalar fields. Such Dirac-Yukawa operators can be decomposed naturally into two terms $\mathcal{D} = \not{\partial}_B + \omega_B$ (subscript B for Bochner) in the same way as one can write the square of the Dirac operator in terms of the Bochner Laplace operator and a

zero-order term $\mathcal{D}^2 = \Delta_B + V_D$. Tolksdorf notices [36] that the action functional

$$\mathcal{D} \mapsto \int_M *tr(V_D)$$

produces the bosonic action of the standard model (as well as the Einstein-Hilbert action) for a suitable generalised Dirac operator of Yukawa type. This construction does not depend on the signature of the metric on M. It is therefore perfectly suitable in the Lorentzian setting.

4 Physical Predictions

Let us now return to the almost-commutative geometry of the standard model. We wish to focus in this section on the constraints for the quartic couplings of the scalar fields, the gauge couplings and the Yukawa couplings.

4.1 Constraints in Parameter Space

Calculating the full spectral action for the standard model is a long and tedious task and we refer to the original publication of Chamseddine and Connes [29] for the details.

The standard model has only one scalar doublet, the Higgs doublet, and only one quartic coupling λ in the Lagrangian. It has three gauge couplings g_1, g_2 and g_3 corresponding to the sub-groups of its structure group $G_{sm} = U(1)\times SU(2)\times SU(3)$. In the almost-commutative setting this structure group arises from Lazzarini's and Schücker's lift of the noncommutative unitaries of the finite algebra $A_f = \mathbb{C} \oplus \mathbb{H} \oplus M(3,\mathbb{C}) \oplus \mathbb{C}$ to the finite Hilbert space.

The finite Dirac operator D_f contains then the Yukawa couplings and the Majorana masses. Calculating the spectral action, normalising the fields and comparing the terms in the a_4 Seeley-DeWitt coefficients leads to the following set of relations at cut-off Λ

$$5\, g_1^2 = 3\, g_2^2 = 3\, g_3^2 = 3\, \frac{Y_2^2}{H}\, \frac{\lambda}{24} = \frac{3}{4}\, Y_2$$

where we Y_2 denotes the trace of the Yukawa matrix squared and H the trace of the Yukawa matrix to the fourth power. The last constraint was first noticed in [30].

4.2 Consequences for the Standard Model

Let us analyse these constraints for the standard model. We need to make some extra assumptions. Namely we will assume the standard model particles constitute the whole particle spectrum, i.e. we have a big desert. Furthermore we take the experimental values of the gauge couplings at the mass of the Z-boson, i.e. $g_1(m_Z) = 0.3575$, $g_2(m_Z) = 0.6514$ and $g_3(m_Z) = 1.221$ [37].

We also assume that the running of the couplings can be described by the standard (1-loop) renormalisation group equations and that the top-quark and the τ-neutrino Yukawa couplings dominate all other Yukawa couplings. We will take $t := \ln(E/m_Z)$, $\mathrm{d}g/\mathrm{d}t =: \beta_g$ and $\kappa := (4\pi)^{-2}$. Then the β-functions are [38, 39]:

$$\beta_{g_i} = \kappa b_i g_i^3, \quad b_i = \left(\tfrac{20}{9}N + \tfrac{1}{6}, -\tfrac{22}{3} + \tfrac{4}{3}N + \tfrac{1}{6}, -11 + \tfrac{4}{3}N\right),$$

$$\beta_t = \kappa \left[-\sum_i c_i^u g_i^2 + Y_2 + \frac{3}{2} g_t^2 \right] g_t,$$

$$\beta_\nu = \kappa \left[-\sum_i c_i^\nu g_i^2 + Y_2 + \frac{3}{2} g_\nu^2 \right] g_\nu,$$

$$\beta_\lambda = \kappa \left[\frac{9}{4} \left(g_1^4 + 2 g_1^2 g_2^2 + 3 g_2^4 \right) - \left(3 g_1^2 + 9 g_2^2 \right) \lambda + 4 Y_2 \lambda - 12 H + 4 \lambda^2 \right],$$

with

$$c_i^t = \left(\tfrac{17}{12}, \tfrac{9}{4}, 8\right), \; c_i^\nu = \left(\tfrac{3}{4}, \tfrac{9}{4}, 0\right),$$
$$Y_2 = 3 g_t^2 + g_\nu^2, \; H = 3 g_t^4 + g_\nu^4.$$

A numerical analysis then shows that $g_2 = g_3$ at $\Lambda = 1.1 \times 10^{17}$ GeV. The constraint discovered by Tolksdorf and Thumstäter results in an upper bound on the top-quark mass, $m_{top} < 190$ GeV. This is in good agreement with experiment, the experimental value of the top-quark mass being $m_{top} = 171.2 \pm 2.1$ GeV. Furthermore no 4th generation of standard model particles is allowed as their masses were forced to be smaller than the top-quark mass and should therefore be detectable.

The numerical analysis can be sharpened using the experimental value of the top-quark mass as an extra input. This allows to calculate the value of the quartic Higgs coupling λ at the cut-off energy and then use the renormalisation group equations to obtain a low energy value. This is the missing ingredient to calculate the Higgs boson mass and one finds $m_H = 168.3 \pm 2.5$ GeV. Unfortunately the Higgs mass has been measured by the LHC to be $m_H \sim 125$ GeV [40], so the almost-commutative standard model is experimentally excluded.

One can also argue that the almost-commutative standard model has excluded before since $\frac{5}{3}\, g_1(\Lambda)^2 \neq g_2(\Lambda)^2$. But this discrepancy has generally been considered as less grim then the exact value of the Higgs mass.

5 Beyond the Standard Model

In view of the failure of the standard model within the setting of almost-commutative geometry as well as the seeming experimental necessity of candidates for dark matter particles it appears to make sense to search for models beyond the standard model.

5.1 Different Approaches

We will focus on some of the ways to construct models that enlarge the particle content of the standard model or change the gauge sector.

The classification scheme of finite spectral triples as proposed by Chamseddine and Connes [21] leads in general to extensions of the gauge sector w.r.t. the standard model gauge group. The simplest viable example is a Pati-Salam type model [22]. Here the symmetry breaking mechanism is far more involved compared to the standard model. This model produces several new scalar fields which may be used to obtain the correct Higgs mass [41].

Another approach with relations to the classification of Chamseddine and Connes was put forward by Devastato, Lizzi and Martinetti [42]. Here the gauge group is enlarged to incorporate also the *Spin*-group and a mixing of spinor degrees of freedom and the finite Hilbert space. This allows to obtain a new scalar field which replaces the Majorana masses of the right-handed neutrinos and also leads to a Higgs mass in accordance with experiment.

A different way to construct particle models was recently revived by Farnsworth and Boyle [43]. They take up an earlier idea of Wulkenhaar [44] which replaces the associative matrix algebras of almost-commutative geometries by non-associative ones. Whether this will lead to interesting models beyond the standard model is still under investigation.

Building on the classification scheme [23] for finite spectral triples we proposed a model building kit where one follows the following steps in order to obtain viable extensions of the standard model:

- find a finite geometry that has the standard model as sub-model (tricky)
  => particle content, gauge group and its representation
- make sure everything is anomaly free
- compute the spectral action => constraints on parameters
- determine the cut-off scale Λ with suitable sub-set of the constraints

- use renormalisation group equations to obtain low energy values of (hopefully) interesting parameters (Higgs couplings, Yukawa couplings)
- check with experiment! (and here we usually fail)

To find a finite spectral triple with the standard model as a sub-geometry, it proved successful to use the finite geometries of standard model type and electro strong type. These can be combined to build bigger finite spectral triples which contain in general new fermions and new gauge bosons. Whether the new model meets all the constraints imposed by further theoretical requirements, such as being free of gauge anomalies, or withstands the confrontation with experiment is often a non-trivial question.

5.2 An Interesting Example

To illustrate viable extensions of the standard model building on the classification [23] we will sketch the model prosed in [26]. The matrix algebra of the internal space is

$$A_f := \mathbb{C} \oplus M_2(\mathbb{C}) \oplus M_3(\mathbb{C}) \oplus \mathbb{C} \oplus_{i=1}^{6} \mathbb{C}_i$$

By a centrally extended lift in the sense of [28] one finds that the structure group of the model is simply the standard model group with an extra $U(1)$ factor. So we have $G_f = U(1)_Y \times SU(2)_w \times SU(3)_c \times U(1)_X$

The finite Hilbert space is extended and has, additionally to the particles of the standard model, the following fermion content in each generation:

$$X_l^1 \oplus X_l^2 \oplus X_l^3 : (0, 1, 1, +1) \oplus (0, 1, 1, +1) \oplus (0, 1, 1, 0)$$

$$X_r^1 \oplus X_r^2 \oplus X_r^3 : (0, 1, 1, +1) \oplus (0, 1, 1, 0) \oplus (0, 1, 1, +1)$$

$$V_\ell^w,\ V_r^w :\ (0, \bar{2}, 1, 0) \quad V_\ell^c,\ V_r^c :\ (-1/6, 1, \bar{3}, 0)$$

where we have given the representations of the structure group and thus the dimension of the subspaces in a short hand notion. So for the V^w particles are in the conjugate of the fundamental representation of the $SU(2)_w$ sub-group and are neutral to all other sub-groups. They also couple vectorially to $SU(2)_w$ (left-right-symmetric) and therefore form a $\mathbb{C}^{24}$ sub-Hilbert space since the anti-particles and three generations have also to be taken into account.

The model has also a new scalar field $\sigma :\ (0, 1, 1, +1)$. We see that all the X-type particles and the new scalar field do not couple to the standard model subgroup while the V-particle have vectorial couplings and therefore their masses should be of the order of the cut-off scale of the effective theory, i.e. the spectral action.

From the spectral action we find the Lagrangians that have to be added to the standard model Lagrangian. For the fermions and the gauge bosons we have

$$\begin{aligned}\mathcal{L}_{ferm} =& g_{\nu,X^1}\,\bar{\nu}_r\sigma X^1_\ell + \bar{X}^1_\ell m_X X^1_r + g_{X^2}\,\bar{X}^2_\ell\sigma X^2_r + g_{X^3}\,\bar{X}^3_\ell\sigma X^3_r \\ &+ \bar{V}^c_\ell m_c V^c_r + \bar{V}^w_\ell m_w V^w_r + \ h.c. \\ \mathcal{L}_{gauge} =& \frac{1}{g_4^2} F^{\mu\nu}_X F_{X,\mu\nu}.\end{aligned}$$

To keep the everything notationally short we only gave the fermionic Lagrangian for one generation. The full Lagrangian contains also CKM-type matrices for the X-particles.

For the scalar sector we write the full potential where we include the Higgs field H:

$$\mathcal{L}_{scalar} = -\mu_1^2|H|^2 - \mu_2^2|\sigma|^2 + \frac{\lambda_1}{6}\,|H|^4 + \frac{\lambda_2}{6}\,|\sigma|^4 + \frac{\lambda_3}{3}\,|H|^2|\sigma|^2$$

Then the symmetry breaking pattern

$$U(1)_Y \times SU(2)_w \times SU(3)_c \times U(1)_X \to U(1)_{e\ell.} \times SU(3)_c \times \mathbb{Z}_2$$

implies that the model has a new massive vector boson associated to the broken $U(1)_X$ sub-group.

So the set of free parameters becomes larger with new Yukawa couplings for the X-particles new quartic couplings λ_2 and λ_3, a new gauge coupling g_4 and Dirac mass terms for the X- and V-particles. But also the set of constraints from the spectral action becomes larger. We find the following boundary conditions on the couplings at the cut-off energy Λ:

$$\begin{aligned} g_2(\Lambda) =& g_3(\Lambda) = \sqrt{\tfrac{7}{6}} \quad g_1(\Lambda) = \sqrt{\tfrac{4}{3}}\, g_4(\Lambda) \\ \lambda_1(\Lambda) =& 36\,\frac{H}{Y_2}\, g_2(\Lambda)^2 \;\; \lambda_2(\Lambda) = 36\,\frac{tr(g^4_{\nu,X^1})}{tr(g^2_{\nu,X^1})^2}\, g_2(\Lambda)^2 \\ \lambda_3(\Lambda) =& 36\,\frac{tr(g^2_\nu)}{Y_2}\, g_2(\Lambda)^2 \\ Y_2(\Lambda) =& tr(g^2_{\nu,X^1})(\Lambda) + tr(g^2_{X^1})(\Lambda) + tr(g^2_{X^2})(\Lambda) = 6\, g_2(\Lambda)^2. \end{aligned}$$

Here $tr(g^2)$ indicates that we take the trace of the corresponding Yukawa matrices (three generations).

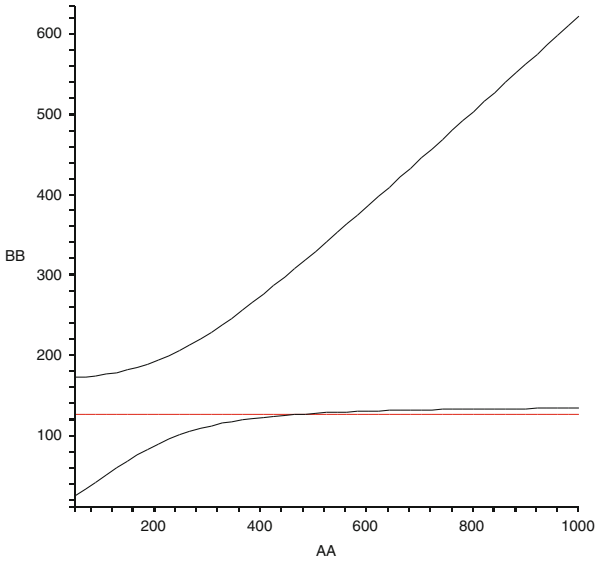


Fig. 1 Mass eigenvalues of the scalar fields

Since these constraints are quite difficult to analyse let us pick a convenient point in the parameter space

$$\begin{aligned} Y_2 \approx & 3g_{top}^2 + g_{\nu_\tau}^2 \\ tr(g_{X^1}^2)(\Lambda) \approx & tr(g_{X^2}^2)(\Lambda) \approx 0 \\ tr(g_{\nu,X^1}^2)(\Lambda) \approx & g_{\nu,X}(\Lambda)^2 = 6\, g_2(\Lambda)^2 \\ (m_{V^w})_{ij} \approx & \Lambda (m_{V^c})_{ij} \approx 10^{15} GeV \end{aligned}$$

where we again assumed that the top-quark and the τ-neutrino Yukawa coupling dominate the Yukawa couplings of the standard model particles.

From a renormalisation group analysis we find then that all of the constraints can be met at $\Lambda \sim 2 \times 10^{18}$ GeV. The masses of the scalar fields do now depend on the three couplings λ_1, λ_2 and λ_3. Their mass matrix is not diagonal anymore and the free parameter in the mass matrix for the mass eigenvalues is the vacuum expectation value of the new scalar field. See Fig. 1 for a plot of the eigenvalues w.r.t. the vacuum expectation value. The straight horizontal line is at 125 GeV, i.e. the mass of the standard model Higgs.

If we require the smaller mass eigenvalue to be the experimental value of the Higgs mass and also put in the experimental value of the top-quark mass with $m_{top} \approx 172.9 \pm 1.5$ GeV we find the following values for the remaining parameters

- $m_{top} \approx 172.9 \pm 1.5$ GeV
- $m_{\sigma_{1,SMS}} \approx 125 \pm 1.1$ GeV

- $m_{\sigma_2} \approx 445 \pm 139\,\text{GeV}$
- $m_{Z_X} \approx 254 \pm 87\,\text{GeV}$
- $g_4(m_Z) \approx 0.36$
- $m_{X_2,X_3} \leq 50\,\text{GeV}$

The quite substantial errors on these predictions originate in the very flat slope of the lower mass eigenvalue, i.e. small errors in the Higgs mass translate into large errors in the second mass eigenvalue and therefore in the other mass terms which depend on it. Whether this model is already excluded is an open question. But such types of models are referred to as *dark sector* models with a *Higgs portal* in the particle physics literature and they seem to be quite difficult to rule out.

6 Challenges for the Future

Let us just mention a couple of challenges and open questions that come into mind in the context of noncommutative geometry and models beyond the standard model.

One of the major open problems in particle physics at the time is probably the lack of mass in the universe. It appears that at least 60 % of the matter we observe astronomically via gravitational effects is unaccounted for by the standard model. So wether models as those discussed above contain viable dark matter candidates seems a pressing question.

On a more fundamental point it is necessary to mention one of the major shortcomings of the almost-commutative approach to the standard model. The "spacetime", i.e. the manifold on which part of the spectral triple is built needs to be of Riemannian signature and has to be compact. This is in stark disagreement with the universe we observe and which we model by a non-compact Lorentzian manifold. For some proposals to solve this problem we refer to Strohmaier [12], Paschke and Sitarz [13], Besnard [14] and Franco and Eckstein [15].

A solution to either of these problems within the context of noncommutative geometry would certainly be a substantial breakthrough.

Acknowledgements The author wishes to thank the organisers of the conference for the kind invitation and the possibility not only to give a talk but also to enjoy so many splendid talks from colleges and interesting discussions.

References

1. https://mediathek.uni-regensburg.de/playthis/547449bcafc7a3.85608488
2. A. Connes, *Noncommutative Geometry* (Academic, San Diego, 1994)
3. A. Connes, M. Marcolli, *Noncommutative Geometry, Quantum Fields and Motives* (American Mathematical Society, Providence, 2008)
4. M. Khalkhali, *Basic Noncommutative Geometry*. EMS Series of Lectures in Mathematics (European Mathematical Society, Zürich, 2010)

5. W. van Suijlekom, *Noncommutative Geometry and Particle Physics* (Springer, Dordrecht, 2015)
6. T. Schücker, Forces from Connes' geometry. Springer Lecture Notes in Physics Lectures 'Topology and Geometry in Physics'. Lect. Notes Phys. **659**, 285–350 (2005)
7. A. Connes, *On the Spectral Characterization of Manifolds* (2008). arXiv:0810.2088 [math.OA]
8. A. Connes, A unitary invariant in Riemannian geometry. Int. J. Geom. Methods Mod. Phys. **5**, 1215–1242 (2008)
9. R. Sanders, *Commutative Spectral Triples and the Spectral Reconstruction Theorem*, Master thesis, University of Nijmegen (2012)
10. F. Pfäffle, C. Stephan, On gravity, torsion and the spectral action principle. J. Funct. Anal. **262**(4), 1529–1565 (2012)
11. A. Sitarz, A. Zajac, Spectral action for scalar perturbations of Dirac operators. Lett. Math. Phys. **98**(3), 333–348 (2011)
12. A. Strohmaier, On noncommutative and pseudo-Riemannian geometry. J. Geom. Phys. **56**(2), 175–195 (2006)
13. M. Paschke, A. Sitarz, Equivariant Lorentzian spectral triples (2006). arXiv preprint math-ph/0611029
14. F. Besnard, A noncommutative view on topology and order. J. Geom. Phys. **59**(7), 861–875 (2009)
15. N. Franco, M. Eckstein, An algebraic formulation of causality for noncommutative geometry. Class. Quantum Gravity **30**(13), 135007 (2013)
16. J. Barrett, A Lorentzian version of the non-commutative geometry of the standard model of particle physics. J. Math. Phys. **48**, 012303 (2007)
17. A. Chamseddine, A. Connes, M. Marcolli, Gravity and the standard model with neutrino mixing. Adv. Theor. Math. Phys. **11**, 991–1089 (2007)
18. C. Stephan, Almost-commutative geometry, massive neutrinos and the orientability axiom in KO-dimension 6 (2006). hep-th/0610097
19. M. Paschke, A. Sitarz, Discrete spectral triples and their symmetries. J. Math. Phys. **39**, 6191 (1998)
20. T. Krajewski, Classification of finite spectral triples. J. Geom. Phys. **28**(1), 1–30 (1998)
21. A. Chamseddine, A. Connes, Why the standard model. J. Geom. Phys. **58**(1), 38–47 (2008)
22. A. Chamseddine, A. Connes, W.D. van Suijlekom, Beyond the spectral standard model: emergence of Pati-Salam unification. J. High Energy Phys. **2013**(11), 1–36 (2013)
23. B. Iochum, T. Schücker, C. Stephan, On a classification of irreducible almost commutative geometries. J. Math. Phys. **45**, 5003 (2004); J.-H. Jureit, C. Stephan, On a classification of irreducible almost commutative geometries, a second helping. J. Math. Phys. **46**, 043512 (2005); T. Schücker, *Krajewski Diagrams and Spin Lifts* (2005). hep-th/0501181; J.-H. Jureit, T. Schücker, C. Stephan, On a classification of irreducible almost commutative geometries III. J. Math. Phys. **46**, 072303 (2005); J.-H. Jureit, C. Stephan, On a classification of irreducible almost commutative geometries IV. J. Math. Phys. **49**, 033502 (2008); J.-H. Jureit, C.A. Stephan, On a classification of irreducible almost-commutative geometries V. J. Math. Phys. **50**, 072301 (2009)
24. C.A. Stephan, Almost-commutative geometries beyond the standard model. J. Phys. A **39**, 9657 (2006); C.A. Stephan, Almost-commutative geometries beyond the standard model II: new colours. J. Phys. A. **40**, 9941 (2007); R. Squellari, C.A. Stephan, Almost-commutative geometries beyond the standard model III: vector doublets. J. Phys. A. **40**, 10685 (2007); C.A. Stephan, New scalar fields in noncommutative geometry. Phys. Rev. **D79**, 065013 (2009)
25. D. Fargion, M.Y. Khlopov, C.A. Stephan, Dark matter with invisible light from heavy double charged leptons of almost-commutative geometry?. Class. Quantum Gravity **23**, 7305–7354 (2006)
26. C.A. Stephan, A dark sector extension of the almost-commutative standard model. Int. J. Mod. Phys. **29**(1), 1450005 (2014)
27. J.-H. Jureit, C.A. Stephan, Finding the standard model of particle physics, a combinatorial problem. Comput. Phys. Commun. **178**, 230–247 (2008)

28. S. Lazzarini, T. Schücker, A farewell to unimodularity. Phys. Lett. B **510**, 277–284 (2001)
29. A. Chamseddine, A. Connes, The spectral action principle. Commun. Math. Phys. **186**(3), 731–750 (1997)
30. T. Thumstädter, *Parameteruntersuchungen an Dirac-Modellen*. PhD- thesis, Universität Mannheim (2003); J. Tolksdorf, T. Thumstädter, Gauge theories of Dirac type. J. Math. Phys. **47**, 082305 (2006); J. Tolksdorf, T. Thumstädter, Dirac type Gauge theories and the mass of the Higgs boson. J. Phys. A. **31**, 9691 (2007)
31. M.A. Kurkov, F. Lizzi, M. Sakellariadou, A. Watcharangkool, Zeta spectral action (2014). arXiv:1412.4669 [hep-th]
32. A.A. Andrianov, M.A. Kurkov, F. Lizzi, Spectral action from anomalies, in *Proceedings of the Corfu Summer Institute on Elementary Particles and Physics – Workshop on Non Commutative Field Theory and Gravity*, Corfu, 8–12 Sept 2010
33. J. Zahn, Locally covariant chiral fermions and anomalies. Nucl. Phys. B **890**, 1 (2015)
34. J. Tolksdorf, The Einstein-Hilbert-Yang-Mills-Higgs action and the Dirac-Yukawa operator. J. Math. Phys. **39**, 2213–2241 (1998)
35. J. Tolksdorf, On the square of first order differential operators of Dirac type and the Einstein-Hilbert action. J. Geom. Phys. **57**(10), 1999–2013 (2007)
36. J. Tolksdorf, The Einstein-Hilbert action with cosmological constant as a functional of generic form (2014). arXiv:1407.3733 [math-ph]
37. K.A. Olive et al., Particle Data Group, Review of particle physics. Chin. Phys. C **38**, 090001 (2014)
38. M.E. Machacek, M.T. Vaughn, Two loop renormalization group equations in a general quantum field theory. 1. Wave function renormalization. Nucl. Phys. B **222**, 83 (1983); 2. Yukawa couplings. Nucl. Phys. B **236**, 221 (1984); 3. Scalar quartic couplings. Nucl. Phys. B **249**, 70 (1985)
39. C. Ford, D.R.T. Jones, P.W. Stephenson, M.B. Einhorn, The effective potential and the renormalisation group. Nucl. Phys. B **395**, 17 (1993)
40. ATLAS Collaboration, Observation of a new particle in the search for the standard model Higgs boson with the ATLAS detector at the LHC. Phys. Lett. B **716**, 1–29 (2012)
41. A. Chamseddine, A. Connes, Resilience of the spectral standard model. J. High Energy Phys. **1209**, 104 (2012)
42. A. Devastato, F. Lizzi, P. Martinetti, Grand symmetry, spectral action, and the Higgs mass (2014). arXiv:1304.0415 [hep-th]
43. L. Boyle, S. Farnsworth, Non-commutative geometry, non-associative geometry and the standard model of particle physics. New J. Phys. **16**, 123027 (2014)
44. R. Wulkenhaar, The standard model within non-associative geometry. Phys. Lett. B **390**, 119–127 (1997)

Variational Stability and Rigidity of Compact Einstein Manifolds

Klaus Kröncke

Contents

Abstract We give a survey on the stability problem of compact Einstein manifolds and on infinitesimal Einstein deformations. We review some important results from this topic, including recent work of the author. Moreover, we discuss applications in mathematical physics.

Keywords Einstein-Hilbert action • Einstein metrics • Variational stability • Infinitesimal Einstein deformations

Mathematics Subject Classification (2010). 53C25, 58E30.

The author thanks the SFB 1085 for financial support.

K. Kröncke (✉)
Fakultät für Mathematik, Universität Regensburg, Universitätsstraße 31, 93059 Regensburg, Germany
e-mail: klaus.kroencke@mathematik.uni-regensburg.de

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3_21

1 Introduction

One of the major aims in Riemannian geometry is to find metrics with nice properties on a given Riemannian manifold. The most common approach to this problem is to detect such metrics as critical points of a geometric functional. Einstein metrics are of particular importance since they satisfy the Einstein equation from general relativity.

Let M^n be a compact manifold of dimension $n \geq 3$ and let $\mathcal{M}$ be the set of smooth Riemannian metrics on it. Einstein metrics can be variationally characterized as critical points of the Einstein-Hilbert action

$$S\colon \mathcal{M} \to \mathbb{R},$$
$$g \mapsto \int_M \mathrm{scal}_g \, dV_g$$

restricted to metrics of some fixed volume [23]. It is well-known that Einstein manifolds are neither local maximum nor minimum of the Einstein-Hilbert action [34]. In fact, both index and coindex of S'' are infinite on any Einstein space. However, there is a notion of stability which is as follows: We say that an Einstein manifold is stable if $S''(h) \leq 0$ for any $h \in \Gamma(S^2M)$ satisfying $\mathrm{tr}h = 0$ and $\delta h = 0$. Such tensors are called transverse traceless. These tensors form the L^2-orhogonal complement of the orbit of the diffeomorphism group acting on the conformal class of g. We call the manifold strictly stable, if $S''(h) < 0$ for all nonzero transverse traceless tensors.

This stability concept plays an important role in mathematical physics. In [1], Andersson and Moncrief proved nonlinear stability (as solutions of the Einstein equation) of Lorentz cones over compact Einstein metrics of negative scalar curvature under the assumption that the compact Einstein metric is stable in the above sense.

Compact Einstein metrics are also used to construct higher-dimensional solutions of the Einstein equation which are considered as background metrics in higher dimensional gravity theories. If the Einstein metric is unstable, there exist linear perturbations of the background which are bounded in space but unbounded in time which suggests nonlinear instability, i.e. small perturbations of initial data for the Einstein equation may yield future incomplete solutions.

The stability condition in the sense of above also plays a role in dynamical stability or instability of Einstein metrics under the Ricci flow. The Ricci flow is a first-order renormalization group flow in string theory, and its solutions are believed to approximate string field theory processes in certain cases. The reason why these stability concepts are deeply connected is that the second variational formulas of Perelman's entropies are given in terms of the Einstein operator.

This survey paper is organized as follows. In Sect. 2, we introduce the notion of stability of compact Einstein manifolds. In Sect. 3, we discuss the above mentioned

applications of this stability concept in mathematical relativity and string theory in more detail.

In the next two sections, we present a variety of results on stability. Stability theorems for Kähler manifolds and for spin manifolds are presented in Sect. 4. In Sect. 5, stability theorems assuming certain bounds on the sectional curvature, the Weyl curvature and the Bochner curvature are given. Finally, Sect. 6 presents some results about infinitesimal Einstein deformations and the moduli space of Einstein structures.

2 The Stability Problem

The second variation of S at Einstein metrics was considered in [26]. For details, see also [3, Chapter 4]. It turned out that S'' admits a block diagonal form with respect to the decomposition

$$T_g\mathcal{M} = \Gamma(S^2M) = C^\infty(M)\cdot g \oplus T_g(g\cdot \mathrm{Diff}(M)) \oplus \mathrm{tr}_g^{-1}(0)\cap \delta_g^{-1}(0). \tag{1}$$

Here, $\delta : \Gamma(S^2M) \to \Omega^1(M)$ denotes the divergence. This decomposition holds for any Einstein metric except the round sphere and all factors are infinite-dimensional.

The first factor of (1) is the tangent space of the conformal class of g. It is known that S'' is positive on volume-preserving conformal deformations. By diffeomorphism invariance, S'' vanishes on the second factor.

The tensors in the third factor are also often called transverse traceless or TT. From now on, we abbreviate $TT_g = \mathrm{tr}_g^{-1}(0)\cap\delta_g^{-1}(0)$. The second variation of S on TT-tensors is given by

$$S''(h) = -\frac{1}{2}\int_M \langle h, \nabla^*\nabla h - 2\mathring{R}h\rangle\, dV.$$

Here, $\mathring{R}$ is the action of the curvature tensor on symmetric $(0,2)$-tensors, given by

$$\mathring{R}h(X,Y) = \sum_{i=1}^n h(R_{e_i,X}Y, e_i).$$

and R is defined with the sign convention such that $\mathring{R}g = \mathrm{Ric}$.

Definition 2.1 We call the operator $\Delta_E : \Gamma(S^2M) \to \Gamma(S^2M)$, given by $\Delta_E h = \nabla^*\nabla h - 2\mathring{R}h$ the Einstein operator.

This is a self-adjoint elliptic operator mapping TT to itself and by compactness of M, it has a discrete spectrum, bounded from below and unbounded from above.

Definition 2.2 We call a compact Einstein manifold (M, g) stable, if the Einstein operator is nonnegative on TT-tensors and strictly stable, if it is positive on TT-tensors. We call (M, g) unstable, if the Einstein operator admits negative eigenvalues on TT. Furthermore, elements in $\ker(\Delta_E|_{TT})$ are called infinitesimal Einstein deformations.

Example The manifolds S^n and $\mathbb{C}P^n$ with their standard metrics are strictly stable. Compact quotients of the hyperbolic space are strictly stable. The flat torus is stable but not strictly stable. The product metric on $S^n \times S^m$ is unstable.

Remark 2.3 Many unstable Einstein manifolds of positive scalar curvature have been explicitly constructed [5, 16, 17, 19, 35, 36]. In contrast, no unstable Einstein manifolds of nonpositive scalar curvature are known.

Question ([9, p. 65]) Are all compact Einstein manifolds with nonpositive scalar curvature stable?

For the Ricci-flat case, this question was already asked by Kazdan and Warner [24, p. 315]. The question can be answered positively in certain cases, see Sect. 4. The statement is not true in the noncompact case since the Riemannian Schwarzschild metric is unstable (see [18, Sec. 5]).

Remark 2.4 If g_t is a nontrivial curve of Einstein metrics through $g = g_0$ orthogonal to $\mathbb{R} \cdot (g \cdot \mathrm{Diff}(M))$, then $\dot{g}_0$ is an infinitesimal Einstein deformation. Evidently, an Einstein manifold is isolated in the space of Einstein structures (the set of Einstein metrics modulo diffeomorphism and rescaling) if $\Delta_E|_{TT}$ has trivial kernel.

Definition 2.5 An infinitesimal Einstein deformation h is called integrable if there exists a curve of Einstein metrics tangent to h.

Given a compact Riemannian manifold (M, g), we call

$$Y(M, [g]) = \inf_{\tilde{g} \in [g]} \mathrm{vol}(M, \tilde{g})^{(2-n)/n} \int_M \mathrm{scal}_{\tilde{g}} \, dV_{\tilde{g}},$$

the Yamabe invariant of the conformal class of g. By the solution of the Yamabe problem, this infimum is always attained by a metric of constant scalar curvature. A metric realizes this infimum is called Yamabe metric. Any Einstein metric is a Yamabe metric. Moreover, any constant scalar curvature metric close to an Einstein metric which is not the round sphere is a Yamabe metric [6, Theorem C].

The set $\mathcal{C}$ of unit-volume constant scalar curvature metrics close to an Einstein metric g is a manifold with tangent space

$$T_g\mathcal{C} = T_g(g \cdot \mathrm{Diff}(M)) \oplus TT$$

and the conformal Yamabe invariant equals the value of the Einstein-Hilbert action on such metrics. Moreover, we have a smooth map

$$\varphi \colon C^\infty(M) \times \mathcal{C} \to \mathcal{M},$$

given by the pointwise multiplication $(f, \tilde{g}) \mapsto f\tilde{g}$, which is a local diffeomorphism around $(1, g)$ [27, Theorem 2.5]. Thus, the map $\tilde{g} \mapsto Y(M, [\tilde{g}])$ is smooth on a neighbourhood of g, g is a critical point and the second variation of Y is only nonvanishing on TT-tensors where it is given by $-(1/2)\Delta_E$. A local stability condition would be to say that g is a local maximum of the Yamabe invariant. It implies the infinitesimal condition in Definition 2.2.

3 Applications in Mathematical Physics

We start this section with a global existence theorem on the Einstein equation, using stability of a compact Einstein metric. In [1], Andersson and Moncrief consider the Lorentz cone

$$\tilde{g} = -dt^2 + \frac{t^2}{n^2} g$$

over a compact $n-$dimensional Riemannian Einstein metric g with normalized scalar curvature $-\frac{n-1}{n}$. The metric $\tilde{g}$ is a Lorentzian Ricci-flat metric, in particular, it solves the Einstein vacuum equations. One may now ask if this solution is stable as a solution of an initial value problem for the Einstein equation.

Observe that the above solution is globally foliated by hypersurfaces of constant mean curvature surfaces $g(t) = (t/n)^2 g$ since the second fundamental form of $g(t)$ is $k(t) = -t^{-1} g(t)$ and thus, the mean curvature is $-n/t$. The CMC-approach is essential in the proof of the following

Theorem 3.1 ([1, Theorem 8.1]) *Let (M, g_0) be a compact Einstein metric of scalar curvature $-\frac{n-1}{n}$. Suppose the Einstein metric is stable in the sense of Definition 2.2 and that all infinitesimal Einstein deformations are integrable.*

Then for any initial data set (g, k) close enough to $(g_0, -n^{-1} g_0)$, the corresponding solution of the Einstein equation is geodesically complete in the future. Moreover, the solution is globally foliated by CMC hypersurfaces and the induced metric on the hypersurfaces converges (up to rescaling) to an Einstein metric close to g_0.

The conditions on the Einstein metric are needed in order to get nice energy estimates. One may also look at the linearized Einstein equation at the background metric $\tilde{g}$. It can be seen that stability is needed to get a nice decay of the linearized perturbations [1, Section 6.4].

Compact Einstein metrics are also used as building blocks for solutions to higher dimensional gravity and supergravity theories. A first example is a product of two Ricci-flat metrics $(M \times N, g \oplus h)$ where (M, g) is a noncompact four-dimensional Lorentzian manifold and (N, h) is some compact Riemannian metric. We now consider solutions of the linearized Einstein equations on the product metric which are of the form $f \cdot k$, where $f \in C^\infty(M)$ and $k \in \Gamma(S^2 N)$. If $\Delta_E h = \lambda k$, f has to

satisfy the Klein-Gordon equation

$$(\Box + m^2)f = 0, \qquad m^2 = \lambda.$$

If $\lambda < 0$, this yields to solutions of the Klein-Gordon equation with imaginary mass and to linear perturbations of the spacetime which are bounded in space but unbounded in time. Therefore, stability in the sense of Definition 2.2 enters naturally as a condition for such spacetimes.

In the context of AdS-CFT correspondence, one considers the so-called Freund-Rubin compactification. Here, we have backgrounds which are of the form $(AdS^5 \times M^5, g_{st} + g)$ where (AdS^5, g_{st}) is the five dimensional standard Anti-de-Sitter space and (M^5, g) is a compact 5-dimensional Riemannian Einstein manifold of positive scalar curvature [15].

We may extend to arbitrary dimensions of the products and consider solutions of the form $(AdS^{n_1} \times M^{n_2}, g_{st} + g)$ with factors being Einstein and the scalar curvatures related by

$$-\frac{n_1 - 1}{n_1}\mathrm{scal}_{g_{st}} = \frac{n_2 - 1}{n_2}\mathrm{scal}_g.$$

Again we look at linear perturbations of the form $f \cdot k$, where $f \in C^\infty(AdS)$ and $k \in \Gamma(S^2M)$. If $\Delta_E h = \lambda k, f$ has again to satisfy the equation

$$(\Box + m^2)f = 0, \qquad m^2 = \lambda.$$

Due to the negative scalar curvature of g_{st}, such a perturbation is considered to be unstable if $m^2 < \frac{n_1-1}{4n_1}\mathrm{scal}_{g_{st}}$ which implies the inequality $\lambda < -\frac{n_2-1}{4n_2}\mathrm{scal}_g$ [7].

Evidently, we call a positive Einstein manifold (M^n, g) physically stable if the smallest eigenvalue of the Einstein operator on TT-tensors satisfies

$$\lambda \geq -\frac{n-1}{4n}\mathrm{scal}_g \tag{2}$$

ore equivalently, the smallest eigenvalue of the Lichnerowicz-Laplacian on TT-tensors satisfies

$$\lambda \geq \frac{\mathrm{scal}_g}{n(n-1)}(4 - \frac{1}{4}(n-5)^2).$$

This condition is also known as the Breitenlohner-Freedman bound.

Another important model in higher-dimensional gravity theory are generalized black holes. Given an Einstein metric (M^n, g) with scalar curvature $n(n-1)$, we can define the Generalised Schwarzschild-Tangherlini spacetimes as

$$-\left(1 - \left(\frac{m}{r}\right)^{n-1}\right)dt^2 + \left(1 - \left(\frac{m}{r}\right)^{n-1}\right)^{-1} dr^2 + r^2 g$$

where m is the mass of the black hole. Observe that one recovers the standard Schwarzschild metric if $(M, g) = (S^2, g_{st})$. These spacetimes are Ricci-flat, so they satisfy the vacuum Einstein equation. We now consider solutions of the linearized Einstein equation which are of the form $e^{\omega t}\varphi(r)r^{-2} \cdot k$ where $k \in \Gamma(S^2M)$ and $\Delta_E k = \lambda k$. By the work in [17], it turned out that if λ violates the Breitenlohner-Freedman bound, we can construct a solution of the above form such that φ is bounded and $\omega \in \mathbb{R}, \omega > 0$. This yields a linear perturbation that is bounded in space but unbounded in time, which is considered as being unstable. It is very interesting that the same eigenvalue bound on the Einstein operator ensures stability in two completely different models.

To conclude this chapter, we discuss applications of stability in studying dynamical stability and instability of Einstein metrics under Ricci flow. Recall that the Ricci flow is a 1-parameter family of metrics satisfying the evolution equation

$$\dot{g}(t) = -2\mathrm{Ric}_{g(t)}.$$

The nonlinear bosonic sigma model is governed by the action

$$E(\phi) = \frac{1}{4\pi\alpha}\int_M \partial_A\phi^i\partial_B\phi^j g_{ij}h^{AB}\, dV_g$$

where (M, g), (N, h) are Riemannian manifolds, $\phi \in C^\infty(M, N)$ and $\alpha > 0$ is a coupling constant. The perturbative quantization of this action yield the renormalization group flow equation

$$\partial_t g_{ij} = -2\alpha\mathrm{Ric}_{ij} - \alpha^2 R_{iklm}R_j^{klm} + O(\alpha^3)$$

and so the Ricci flow equation appears as the first loop order term of this renormalization group flow. Connections between Ricci flow and renormalization group flow have been investigated a lot, see e.g. [8]. Ricci flow has been used in the context of stability of black holes and of anti de Sitter space, see [13, 22, 38].

The fixed points of the volume-normalized Ricci flow (which is more common in the context of compact manifolds) are Einstein metrics. It is now natural to ask how the Ricci flow behaves as a dynamical system close to an Einstein metric.

We present recent dynamical stability and instability theorems which are closely related to the stability concept above. In the Ricci-flat case, the theorems are due to Haslhofer whereas in the case of positive and negative scalar curvature, the results were obtained by the author.

Theorem 3.2 ([20, Theorem F],[31, Theorems 5.4.13 and 6.4.7]) *Let (M, g) be a compact Einstein manifold with Einstein constant μ such that the Einstein operator is nonnegative on TT-tensors, the smallest nonzero eigenvalue of the Laplacian satisfies $\lambda > 2\mu$ and all infinitesimal Einstein deformations are integrable. Let $k \geq 3$.*

Then for every C^k-neighbourhood $\mathcal{U}$ of g, there exists a smaller C^{k+2}-neighbourhood $\mathcal{V} \subset \mathcal{U}$ of g such that any (volume-)normalized Ricci flow starting in $\mathcal{V}$ stays in $\mathcal{U}$ for all time and converges exponentially fast to some Einstein metric $g_\infty \in \mathcal{U}$ as $t \to \infty$.

Theorem 3.3 ([20, Theorem F],[31, Theorems 5.4.14 and 6.4.8]) *Let (M, g) be an Einstein manifold with constant μ and suppose that all infinitesimal Einstein deformations are integrable. If the Einstein operator admits negative eigenvalues or there is a Laplace eigenvalue contained in $(0, 2\mu)$, then there exists a nontrivial ancient normalized Ricci flow emerging from it, i.e. there is a Ricci flow $g(t)$, $t \in (-\infty, 0]$ such that $\lim_{t\to-\infty} g(t) = g$.*

Remark 3.4 The integrability condition can also be dropped. In this case, the conditions on the Einstein operator in both theorems are replaced by the condition that g is a local maximum of the Yamabe invariant (for dynamical stability) or that it is not a local maximum of the Yamabe invariant (for dynamical instability). As consequences, we possibly have to pull back the flow by diffeomorphisms to make it convergent and the convergence speed is just polynomially. In in particular, any Einstein metric is either dynamically stable or dynamically unstable. For details, see [21, 30].

Remark 3.5 Various dynamical stability results have also been proven in the noncompact case [2, 12, 37]. In this case, there are some subtleties concerning the falloff conditions of perturbations at infinity. All in all, the results are much less complete than in the compact case.

4 Stability and Additional Geometric Structures

In this section, we discuss some stability results from the literature which assume the presence of additional geometric structures. Moreover, we sketch how these structures are used in the proofs.

Theorem 4.1 ([11, Corollary 1.2]) *Any Kähler-Einstein manifold of nonpositive scalar curvature is stable.*

The proof idea is essentially due to [29]. It turned out that the Einstein operator preserves hermitian and skew-hermitian tensors. If h is hermitian, we define a 2-form by $\phi(X, Y) = h \circ J(X, Y) := h(X, J(Y))$ and

$$\Delta_H \phi = (\Delta_E h) \circ J + 2\mu\phi, \tag{3}$$

where Δ_H is the Hodge Laplacian on 2-forms and μ is the Einstein constant. If h is skew-hermitian, we define a symmetric endomorphism $I : TM \to TM$ by

$$g \circ I = h \circ J,$$

and since $IJ + JI = 0$, we may consider I as a $T^{1,0}M$-valued 1-form of type $(0, 1)$. We have the formula

$$g \circ (\Delta_C I) = (\Delta_E h) \circ J, \tag{4}$$

where Δ_C is the complex Laplacian. The assertion now follows from the fact that Δ_H and Δ_C are nonnegative.

Since any Ricci-flat Kähler-metric carries a parallel spinor and any negative Kähler-Einstein manifold carries a parallel spin^c spinor, Theorem 4.1 follows from Theorems 4.2 and 4.4 below. However, the above formulas allow us to compute the space of infinitesimal Einstein deformations in terms of cohomology classes. We discuss this in more detail in Sect. 6.

Theorem 4.2 ([41, Proposition 2.4], [10, Theorem 1.1]) *Let (M, g) be a compact Ricci-flat spin manifold carrying a parallel spinor. Then (M, g) is stable.*

The idea is as follows: Given a parallel spinor, we associate to each symmetric $(0, 2)$-tensor a spinor-valued 1-form by

$$\begin{aligned} \Psi\colon \Gamma(S^2M) &\to \Gamma(T^*M \otimes S), \\ h &\mapsto (X \mapsto h(X) \cdot \sigma). \end{aligned}$$

Here, S denotes the spinor bundle of (M, g) and h is considered as an endomorphism on TM. Now a straightforward calculation shows that if $h \in TT$,

$$D^2 \circ \Psi(h) = \Psi \circ \Delta_E(h)$$

for any TT-tensor g. Here, D is the twisted Dirac operator acting on the space $\Gamma(T^*M \otimes S)$. Since D^2 is a nonnegative operator, (M, g) is stable.

Now assume that the manifold is spin and there exists a real Killing spinor σ, i.e. $\nabla_X \sigma = cX \cdot \sigma$ for some $c \in \mathbb{R}$, $c \neq 0$. Any Riemannian manifold carrying a real Killing spinor is Einstein with constant $4c^2(n-1)$. For such manifolds, stability can not longer be derived but a weaker result holds:

Theorem 4.3 ([17, Section 4.3]) *Let (M, g) be a positive Einstein manifold which is spin. If (M, g) carries a real Killing spinor, it is physically stable (i.e. stable in the sense of the eigenvalue bound (2)).*

The prove is similar as above. Using the Killing spinor σ, we can define the map Ψ as above and we get

$$(D - c)^2 \circ \Psi(h) = \Psi \circ \Delta_E(h) + c^2(n-1)^2 \Psi(h).$$

where c is the Killing constant. Thus, the smallest eigenvalue of $\Delta_E|_{TT}$ is bounded from below by $-\frac{n-1}{4}\mu$ where $\mu > 0$ is the Einstein constant. To finish this section, we mention a stability theorem in the spin^c-case:

Theorem 4.4 ([11, Theorem 1.1]) *Let (M, g) be a spin^c Einstein manifold with nonpositive scalar curvature. If (M, g) admits a parallel spin^c spinor, it is stable.*

Having a parallel spin^c spinor σ, one defines Ψ as above, but now it is a map $\Psi\colon \Gamma(S^2M) \to \Gamma(T^*M \otimes S^c)$ where S^c is the spin^c spinor bundle. The Bochner formula reads

$$D^2 \circ \Psi(h) = \Psi \circ \Delta_E(h) + \Psi(\mathrm{Ric} \circ h) - \Psi(h \circ F),$$

where F is the curvature form of the line bundle of the spin^c structure. It can be shown now that

$$\mathrm{Re}\langle \Psi(\mathrm{Ric} \circ h) - \Psi(h \circ F), \Psi(h)\rangle \leq 0$$

which implies that Δ_E does not have negative eigenvalues.

5 Stability Under Curvature Conditions

The first stability criterion formulated in terms of curvature conditions was proven by Koiso. Let the function $r : M \to \mathbb{R}$ by be defined as

$$r(p) = \sup \left\{ \frac{\langle \mathring{R}\eta, \eta\rangle_p}{|\eta|_p^2} \;\middle|\; \eta \in (S^2M)_p, \mathrm{tr}_g(\eta) = 0 \right\}. \tag{5}$$

Theorem 5.1 ([25, Theorem 3.3]) *Let (M, g) be an Einstein manifold with Einstein constant μ which satisfies*

$$\sup_{p\in M} r(p) \leq \max\left\{-\mu, \frac{1}{2}\mu\right\}.$$

Then (M, g) is stable. If the strict inequality holds, then (M, g) is strictly stable.

The proof is based on the Bochner technique. For the Einstein operator, we have the formulas

$$(\Delta_E h, h)_{L^2} = \|D_1 h\|_{L^2}^2 + 2\mu \|h\|_{L^2}^2 - 4(\mathring{R}h, h)_{L^2} - 2\|\delta h\|_{L^2}^2, \tag{6}$$

$$(\Delta_E h, h)_{L^2} = \|D_2 h\|_{L^2}^2 - \mu \|h\|_{L^2}^2 - (\mathring{R}h, h)_{L^2} + \|\delta h\|_{L^2}^2, \tag{7}$$

where the two differential operators D_1 and D_2 are given by

$$D_1 h(X, Y, Z) = \frac{1}{\sqrt{3}}(\nabla_X h(Y, Z) + \nabla_Y h(Z, X) + \nabla_Z h(X, Y)),$$

$$D_2h(X,Y,Z) = \frac{1}{\sqrt{2}}(\nabla_X h(Y,Z) - \nabla_Y h(Z,X)).$$

The result now follows quite immediately.

One can estimate r in a purely algebraic way in terms of sectional curvature bounds and one gets the following corollaries as consequences thereof:

Corollary 5.2 (Bourguignon, unpublished) *Let (M,g) be an Einstein manifold such that the sectional curvature lies in the interval $(\frac{n-2}{3n}, 1]$. Then (M,g) is strictly stable.*

Corollary 5.3 ([25, Proposition 3.4]) *Let (M,g) be an Einstein manifold with sectional curvature $K < 0$. Then (M,g) is strictly stable.*

In our work, we used the fact that the curvature tensor of any Einstein metric admits the decomposition

$$R = W + \frac{\mu}{2(n-1)} g \owedge g, \tag{8}$$

where μ is the Einstein constant of g and $\owedge$ denotes the Kulkarni-Nomizu product of 2-tensors. The tensor W is the Weyl curvature tensor. Let

$$w(p) = \sup \left\{ \frac{\langle \mathring{W}\eta, \eta\rangle_p}{|\eta|_p^2} \;\middle|\; \eta \in (S^2M)_p = 0 \right\}, \tag{9}$$

where $\mathring{W}h(X,Y) = \sum_{i=1}^n h(W(e_i,X)Y,e_i)$. The operator $\mathring{W} \in \mathrm{End}(S^2M)$ is trace-free at each point $p \in M$ and therefore, $w \geq 0$. Using the Bochner formulas from above, we can prove

Theorem 5.4 ([33, Theorem 1.4]) *An Einstein manifold (M,g) with constant μ is stable if*

$$\|w\|_{L^\infty} \leq \max\left\{ \mu\frac{n+1}{2(n-1)}, -\mu\frac{n-2}{n-1} \right\}.$$

If the strict inequality holds, then (M,g) is strictly stable.

This theorem shows that if the Weyl tensor is small enough at each point, the manifold is stable. However, we were also able to prove a criterion involving an integral of the function w:

Theorem 5.5 ([33, Theorem 1.5]) *Let (M,g) be an Einstein manifold with positive Einstein constant μ. If*

$$\|w\|_{L^{n/2}} \leq \mu \cdot \mathrm{vol}(M,g)^{2/n} \cdot \frac{n+1}{2(n-1)} \left(\frac{4(n-1)}{n(n-2)} + 1 \right)^{-1},$$

then (M, g) is stable. If the strict inequality holds, then (M, g) is strictly stable.

Observe that for large dimensions, the two above conditions are close to each other. The main tool we use for the second criterion is the Sobolev inequality

$$4\frac{n-1}{n-2}\|\nabla f\|_{L^2}^2 \geq \operatorname{scal}\left\{\|f\|_{L^{\frac{2n}{n-2}}}^2 - \|f\|_{L^2}^2\right\}, \tag{10}$$

which holds for any unit-volume Yamabe metric and any $f \in H^1(M)$. It is not hard to see that the Sobolev inequality also holds for tensor fields. The proof follows from an optimal combination of (6), (10) and the Hölder inequality.

As is well-known, the Weyl tensor is conformally invariant. It is then not hard to show that the $L^{n/2}$-norm of w is conformally invariant. This allows us to deduce

Corollary 5.6 ([33, Corollary 3.7]) *Let (M, g) be a Riemannian manifold and let $Y([g])$ be the Yamabe constant of the conformal class of g. If*

$$\|w\|_{L^{n/2}(g)} \leq Y([g])\frac{n+1}{2n(n-1)} \cdot \left(\frac{4(n-1)}{n(n-2)} + 1\right)^{-1}, \tag{11}$$

any Einstein metric in the conformal class of g is stable.

In dimension 6, we also proved a stability criterion involving the Euler characteristic.

Theorem 5.7 ([33, Theorem 1.6]) *Let (M, g) be a positive Einstein six-manifold with constant μ and $\operatorname{vol}(M, g) = 1$. If*

$$\frac{1}{25}\left(144 - \frac{12 \cdot 7^2 \cdot 3^2}{5 \cdot 11^2}\right)\mu^3 \leq 384\pi^3\chi(M) - 48\int_M \operatorname{tr}(\hat{W}^3)\, dV,$$

then (M, g) is strictly stable. Here, $\hat{W}$ is the Weyl curvature operator acting on two-forms.

Here, the proof follows from the Gauss-Bonnet formula in dimension six, a Bochner-type formula for the Laplacian of the Weyl-tensor and Theorem 5.5.

In the Kähler-Einstein case, the Bochner-tensor B measures the deviation of the manifold of being of constant holomorphic sectional curvature. Similarly as above, we can also prove stability criterions involving the Bochner tensor. We introduce the function

$$b(p) = \sup\left\{\frac{\langle \mathring{B}\eta, \eta\rangle}{|\eta|^2} \,\middle|\, \eta \in (S^2M)_p\right\}, \tag{12}$$

where $\mathring{B}h(X, Y) = \sum_{i=1}^n h(B(e_i, X)Y, e_i)$. Using a decomposition of the curvature tensor in the Kähler case, we can prove

Theorem 5.8 ([33, Theorem 5.6]) *Let (M, g, J) be Kähler-Einstein with positive Einstein constant μ. If*

$$\|b\|_{L^\infty} \leq \frac{\mu(n-2)}{2(n+2)},$$

then (M, g) is stable.

As in the Weyl tensor case, we can also use the Sobolev inequality to prove an integral criterion:

Theorem 5.9 ([33, Theorem 5.7]) *Let (M, g, J) be a positive Kähler-Einstein manifold with constant μ. If the function b satisfies*

$$\|b\|_{L^{n/2}} \leq \mu \cdot \mathrm{vol}(M, g)^{2/n} \cdot \frac{(n-2)}{2(n+2)} \left(\frac{4(n-1)}{n(n+2)} + 1 \right)^{-1},$$

then (M, g) is stable.

6 Infinitesimal Einstein Deformations

Let $g \in \mathcal{M}$ be Einstein with Einstein constant μ and volume $c > 0$ and let $\mathcal{E}$ the set of all Einstein metrics on a fixed manifold. We are interested in the structure of the set of Einstein structures, that is the image of $\mathcal{E}$ under the quotient map $\varphi : \mathcal{M} \to \mathcal{M}/\mathrm{Diff}(M)$.

An appropriate tool to describe this set is provided by Ebin's slice theorem [14, Theorem 7.1], which states the existence of a local slice of the quotient map φ. More precisely, we have a smooth submanifold $\mathcal{S} \subset \mathcal{M}$ with tangent space $\delta^{-1}(0)$ and any metric close to g is isometric to a unique metric in $\mathcal{S}$.

Now, let us discuss the result of [29, Theorem 3.1]: There exists an analytic finite-dimensional submanifold $\mathcal{Z}$ of $\mathcal{S}$ such that $T_g\mathcal{Z} = \ker(\Delta_E|_{TT})$ and $\mathcal{F} := \{\tilde{g} \in \mathcal{E} \cap \mathcal{S} \mid \mathrm{vol}(\tilde{g}) = c\}$ is an analytic subset of $\mathcal{Z}$. If all infinitesimal Einstein deformations are integrable, we may choose $\mathcal{S}$ and $\mathcal{Z}$ such that $\mathcal{F} = \mathcal{Z}$. In particular, the moduli space of Einstein structures close to g is a manifold in this case.

If (M, g) is a product of surfaces (Σ_i, g_i) $i = 1, 2$ with hyperbolic metrics, $\mathcal{F}$ is a manifold which is locally diffeomorphic to the product of the Teichmüller spaces of Σ_1 and Σ_2. By choosing surfaces of high genus, we can easily construct Einstein metrics whose moduli space of Einstein structures is locally of arbitrary large dimension [1, Section 3.4].

In the Kähler case, there exists an important result which allows to compute the dimension of $\ker(\Delta_E|_{TT})$ for many examples.

Proposition 6.1 ([29, Corollary 9.4]) *Let (M, g, J) be a Kähler-Einstein manifold. Then we have*

$$\begin{aligned}
\dim(\ker(\Delta_E|_{TT}) &= 2\dim_{\mathbb{C}} H^1(M,\Theta) && \text{if } \mathrm{scal}_g < 0;\\
\dim(\ker(\Delta_E|_{TT}) &= \dim_{\mathbb{R}} H^{1,1}(M,J) - 1 \\
&\quad + 2(\dim_{\mathbb{C}} H^1(M,\Theta) - \dim_{\mathbb{C}} H^{0,2}(M,J)) && \text{if } \mathrm{scal}_g = 0;\\
\dim(\ker(\Delta_E|_{TT}) &\geq 2\dim_{\mathbb{C}} H^1(M,\Theta) && \text{if } \mathrm{scal}_g > 0;
\end{aligned}$$

where Θ is the sheaf of holomorphic vector fields.

The proof basically relies on (3) and (4). By the Bogomolov-Tian-Todorov theorem [4, 39, 40], all infinitesimal Einstein deformations are integrable in the Calabi-Yau case. In other words the moduli space of Calabi-Yau metrics (which equals the space of Einstein metrics in a small neighbourhood of g) forms a smooth manifold whose dimension can be explicitly computed. For example, its dimension is 57 in the case of the K3 surface.

Let us turn to a different case where the dimension can be explicitly computed: We consider are flat connected compact manifolds, which are called Bieberbach manifolds. It is well known that any Bieberbach manifold is isometric to $\mathbb{R}^n/G$, where G is a suitable subgroup of the Euclidean motions $E(n) = O(n) \ltimes \mathbb{R}^n$. On Bieberbach manifolds, we can explicitly compute the dimension of the space of infinitesimal Einstein deformations.

Theorem 6.2 ([32, Theorem 1.1]) *Let $(M = \mathbb{R}^n/G, g)$ be a Bieberbach manifold and let ρ be the canonical representation of the holonomy of G on $\mathbb{R}^n$. Let*

$$\rho \cong (\rho_1)^{i_1} \oplus \ldots \oplus (\rho_l)^{i_l}$$

be an irreducible decomposition of ρ. Then the dimension of the space of infinitesimal Einstein deformations is equal to

$$\dim(\ker(\Delta_E|_{TT})) = \sum_{j=1}^{l} \frac{i_j(i_j+1)}{2} - 1.$$

We use the fact that $\ker(\Delta_E|_{TT})$ coincides with the space of parallel traceless symmetric 2-tensors whose computation can be computed using holonomy theory. All these deformations are integrable since the map $t \mapsto g + th$ generates a family of flat metrics if h is parallel. In particular, all Ricci-flat metrics close to a flat metric are also flat.

Let us now turn to the case of product manifolds. Let (M, g_1) and (N, g_2) be Einstein manifolds. If both manifolds have the same Einstein constant, the product manifold $(M \times N, g_1 + g_2)$ is also Einstein and we may ask how the moduli space

of Einstein metrics on the product manifold is related to the moduli spaces of the factors.

Andersson and Moncrief studied products of negative Einstein manifolds. They showed the following: Let $\mathcal{E}_\mu(M)$ and $\mathcal{E}_\mu(N)$ be the sets of Einstein metrics of constant μ on M, N, respectively. Let (M, g_1) and (N, g_2) both be stable Einstein manifolds of negative Einstein constant μ and suppose, all infinitesimal Einstein deformations are integrable, there exist slices $\mathcal{S}(M)$, $\mathcal{S}(N)$ and $\mathcal{S}(M \times N)$ of the spaces of metrics in M, N and $M \times N$ such that

$$\mathcal{E}_\mu(M \times N) \cap \mathcal{S}(M \times N) \cong (\mathcal{E}_\mu(M) \cap \mathcal{S}(M)) \times (\mathcal{E}_\mu(N) \cap \mathcal{S}(N)), \tag{13}$$

see [1, Corollary 3.4]. In particular,

$$\dim(\ker(\Delta_E^{M\times N}|_{TT}) = \dim(\ker(\Delta_E^N|_{TT}) \oplus \dim(\ker(\Delta_E^N|_{TT}). \tag{14}$$

In [32], we discussed the same questions for Ricci-flat and positive stable Einstein metrics under the same stability and integrability assumptions. We showed that in the Ricci-flat case, (13) and (14) do not longer hold if both factors admit parallel vector fields. If X, Y are parallel vector fields on M, N, respectively, the symmetric tensor product $h = X \odot Y$ is an infinitesimal Einstein deformation which is integrable.

In the case of positive scalar curvature, there exists a large class of examples where (14) is violated. If f is a smooth function on one of the factors such that $\Delta f = 2\mu f$ where μ is the Einstein constant, then for appropriate parameters $\alpha, \beta, \gamma \in \mathbb{R}$ not all equal to zero, the tensor

$$\alpha f \cdot g_1 + \beta f \cdot g_2 + \nabla^2 f \tag{15}$$

is a TT-tensor which is in the kernel of the Einstein operator. For Kähler-Einstein manifolds, $2\mu \in \mathrm{spec}_+(\Delta)$ if and only if the manifold admits a holomorphic vector field. This holds for all known examples of Kähler-Einstein metrics.

On $S^2 \times \mathbb{C}P^{2n}$ there exist infinitesimal Einstein deformations which are all of the above form. In [28], it was shown that they are all not integrable and both sides of (13) consist of a point in this case. It is not known, whether general deformations of the form in (15) can be integrable and whether (13) can be violated.

References

1. L. Andersson, V. Moncrief, Einstein spaces as attractors for the Einstein flow. J. Differ. Geom. **89**(1), 1–47 (2011)
2. R. Bamler, Stability of symmetric spaces of noncompact type under Ricci flow. Geom. Funct. Anal. **25**(2), 342–416 (2015)
3. A.L. Besse, *Einstein Manifolds*. Reprint of the 1987 edition (Springer, Berlin, 2008)
4. F.A. Bogomolov, Hamiltonian Kähler manifolds. Sov. Math. Dokl. Bd. **19**, 1462–1465 (1978)

5. C. Böhm, Unstable Einstein metrics. Math. Z. **250**(2), 279–286 (2005)
6. C. Böhm, M.Y. Wang, W. Ziller, A variational approach for compact homogeneous Einstein manifolds. Geom. Funct. Anal. **14**(4), 681–733 (2004)
7. P. Breitenlohner, D.Z. Freedman, Positive energy in anti-de Sitter backgrounds and gauged extended supergravity. Phys. Lett. B **115**(3), 197–201 (1982)
8. M. Carfora, Renormalization group and the Ricci flow. Milan J. Math. **78**(1), 319–353 (2010)
9. X. Dai, Stability of Einstein metrics and spin structures, in *Proceedings of the 4th International Congress of Chinese Mathematicians*, Hangzhou, vol. II (2007), pp. 59–72
10. X. Dai, X. Wang, G. Wei, On the stability of Riemannian manifold with parallel spinors. Invent. Math. **161**(1), 151–176 (2005)
11. X. Dai, X. Wang, G. Wei, On the variational stability of Kähler-Einstein metrics. Commun. Anal. Geom. **15**(4), 669–693 (2007)
12. A. Deruelle, Stability of non compact steady and expanding gradient Ricci solitons (2014, preprint). arXiv:1404.2390
13. S. Dutta, V. Suneeta, Investigating stability of a class of black hole spacetimes under Ricci flow. Class. Quant. Gravity **27**(7), 075012 (2010)
14. D.G. Ebin, The manifold of Riemannian metrics. Proc. Symp. AMS Bd. **15**, 11–40 (1970)
15. P.G.O. Freund, M.A. Rubin, Dynamics of dimensional reduction. Phys. Lett. B **97**(2), 233–235 (1980)
16. G.W. Gibbons, S.A. Hartnoll, Gravitational instability in higher dimensions. Phys. Rev. D **66**(6), 064024 (2002)
17. G.W. Gibbons, S.A. Hartnoll, C.N. Pope, Bohm and Einstein-Sasaki metrics, black holes, and cosmological event horizons. Phys. Rev. D **67**(8), 84024 (2003)
18. D.J. Gross, M.J. Perry, Instability of flat space at finite temperature. Phys. Rev. D **25**(2), 330–355 (1982)
19. S.S. Gubser, I. Mitra, Some interesting violations of the Breitenlohner-Freedman bound. J. High Energy Phys. **2002**(7), 044 (2002)
20. R. Haslhofer, Perelman's lambda-functional and the stability of Ricci-flat metrics. Calc. Var. Partial Differ. Equ. **45**(3–4), 481–504 (2012)
21. R. Haslhofer, R. Müller, Dynamical stability and instability of Ricci-flat metrics. Math. Ann. **360**(1–2), 547–553 (2014)
22. M. Headrick, T. Wiseman, Ricci flow and black holes. Class. Quant. Gravity **23**(23), 6683 (2006)
23. D. Hilbert, Die Grundlagen der Physik. (Erste Mitteilung.). Gött. Nachr. 395–407 (1915)
24. J.L. Kazdan, F.W. Warner, Prescribing curvatures, in *Differential Geometry. Proceedings of Symposia in Pure Mathematics*, Stanford, vol. 27, Part 2 (1975)
25. N. Koiso, Non-deformability of Einstein metrics. Osaka J. Math. **15**, 419–433 (1978)
26. N. Koiso, On the second derivative of the total scalar curvature. Osaka J. Math. **16**, 413–421 (1979)
27. N. Koiso, A decomposition of the space $\mathcal{M}$ of Riemannian metrics on a manifold. Osaka J. Math. **16**, 423–429 (1979)
28. N. Koiso, Rigidity and infinitesimal deformability of Einstein metrics. Osaka J. Math. **19**, 643–668 (1982)
29. N. Koiso, Einstein metrics and complex structures. Invent. Math. **73**, 71–106 (1983)
30. K. Kröncke, Ricci flow, Einstein metrics and the Yamabe invariant (2013, preprint). arXiv:1312.2224
31. K. Kröncke, *Stability of Einstein Manifolds.* PhD thesis, Universität Potsdam (2013)
32. K. Kröncke, On infinitesimal Einstein deformations. Differ. Geom. Appl. **38**, 41–57 (2015)
33. K. Kröncke, On the stability of Einstein manifolds. Ann. Glob. Anal. Geom. **47**(1), 81–98 (2015)
34. Y. Muto, On Einstein metrics. J. Diff. Geom. **9**(4), 521–530 (1974)
35. D.N. Page, C.N. Pope, Stability analysis of compactifications of D = 11 supergravity with SU(3)×SU(2)×U(1) symmetry. Phys. Lett. **145**(5), 337–341 (1984)

36. D.N. Page, C.N. Pope, Which compactifications of D = 11 supergravity are stable? Phys. Lett. **144**(5–6), 346–350 (1984)
37. O. Schnürer, F. Schulze, M. Simon, Stability of Euclidean space under Ricci flow. Commun. Anal. Geom. **16**(1), 127–158 (2008)
38. V. Suneeta, Investigating off-shell stability of anti-de Sitter space in string theory. Class. Quant. Gravity **26**(3), 035023 (2009)
39. G. Tian, Smoothness of the universal deformation space of compact Calabi-Yau manifolds and its Petersson-Weil metric. Math. Asp. String Theory **1**, 629–646 (1987)
40. A.N. Todorov, The Weil-Petersson geometry of the moduli space of SU(n$\geq$ 3) (Calabi- Yau) manifolds. I. Commun. Math. Phys. **126**(2), 325–346 (1989)
41. M.Y. Wang, Preserving parallel spinors under metric deformations. Indiana Univ. Math. J. **40**(3), 815–844 (1991)
42. R. Ye, Ricci flow, Einstein metrics and space forms. Trans. Am. Math. Soc. **338**(2), 871–896 (1993)

Index

F. Finster et al. (eds.), *Quantum Mathematical Physics*,
DOI 10.1007/978-3-319-26902-3